

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
 Data File : BF123923.D
 Acq On : 12 May 2021 14:36
 Operator : JU/CG
 Sample : M2340-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EFF-WW

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123923.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.357	545	556	563	rBV2	6202776	15088045	6.95%	2.711%
2	5.516	578	583	586	rVB	5556885	6053379	2.79%	1.088%
3	5.593	591	596	602	rBV	5219205	7683958	3.54%	1.381%
4	5.746	619	622	625	rVB	3356725	2833923	1.31%	0.509%
5	5.910	645	650	652	rBV	8204060	7838669	3.61%	1.408%
6	6.516	748	753	756	rBV	4261694	4560665	2.10%	0.819%
7	7.004	797	836	839	rVV2	22894583	217083917	100.00%	39.003%
8	7.222	870	873	888	rVB2	1381158	2664065	1.23%	0.479%
9	7.345	888	894	897	rVB	3836664	4003556	1.84%	0.719%
10	7.404	899	904	907	rVB	11180690	12313115	5.67%	2.212%
11	7.534	907	926	929	rBV	8624732	11689578	5.38%	2.100%
12	7.687	929	952	956	rVB3	4486612	25834207	11.90%	4.642%
13	7.963	980	999	1000	rBV3	3127321	10804584	4.98%	1.941%
14	8.645	1111	1115	1118	rVB	4430171	3426513	1.58%	0.616%
15	9.128	1190	1197	1204	rBV	6536797	6569312	3.03%	1.180%
16	9.798	1305	1311	1315	rBV2	2264971	2209951	1.02%	0.397%
17	10.586	1440	1445	1451	rVB2	2294654	2361971	1.09%	0.424%
18	10.851	1484	1490	1491	rBV	13860618	22012780	10.14%	3.955%
19	10.886	1492	1496	1498	rVV	19122171	35718548	16.45%	6.417%
20	10.910	1498	1500	1522	rVB	16015412	37198570	17.14%	6.683%
21	11.286	1561	1564	1581	rVB	2137002	2581811	1.19%	0.464%
22	12.380	1746	1750	1755	rVV2	2755303	3850888	1.77%	0.692%
23	12.598	1783	1787	1788	rVV	1985844	2265145	1.04%	0.407%
24	12.639	1788	1794	1797	rVV2	6414429	8701346	4.01%	1.563%
25	12.722	1804	1808	1810	rVV	3944474	4178313	1.92%	0.751%
26	12.822	1821	1825	1830	rBV	5413348	5608606	2.58%	1.008%
27	12.874	1830	1834	1837	rVV	4385702	4454686	2.05%	0.800%
28	13.104	1870	1873	1877	rBV	3056107	2893942	1.33%	0.520%
29	13.192	1884	1888	1891	rVV	4810721	4566338	2.10%	0.820%
30	13.545	1945	1948	1953	rVB	3296433	3320287	1.53%	0.597%
31	13.798	1976	1991	1993	rBV	13478111	20218887	9.31%	3.633%
32	13.892	2003	2007	2009	rBV	2563090	2393105	1.10%	0.430%
33	14.410	2091	2095	2098	rVB	10103923	9950518	4.58%	1.788%
34	15.045	2198	2203	2206	rBV2	3376522	4546449	2.09%	0.817%
35	15.080	2206	2209	2225	rVB2	4115033	11969790	5.51%	2.151%
36	18.086	2692	2720	2722	rBV	6747933	24634534	11.35%	4.426%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.886	2846	2856	2866	rVB2	787538	2497768	1.15%	0.449%
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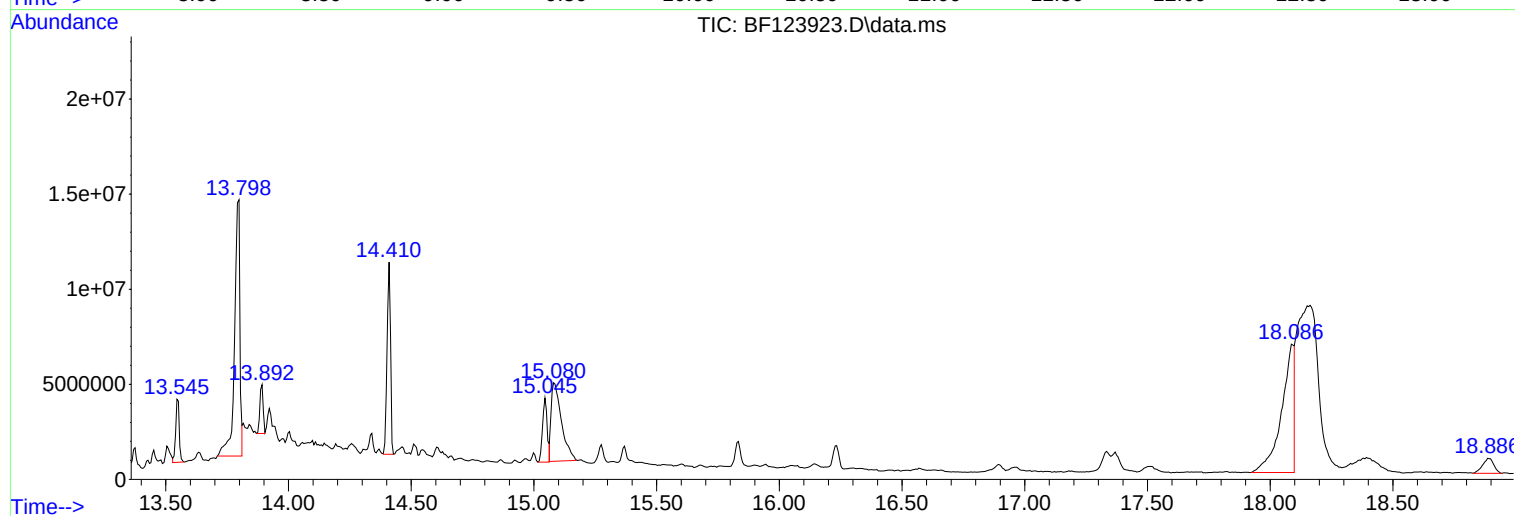
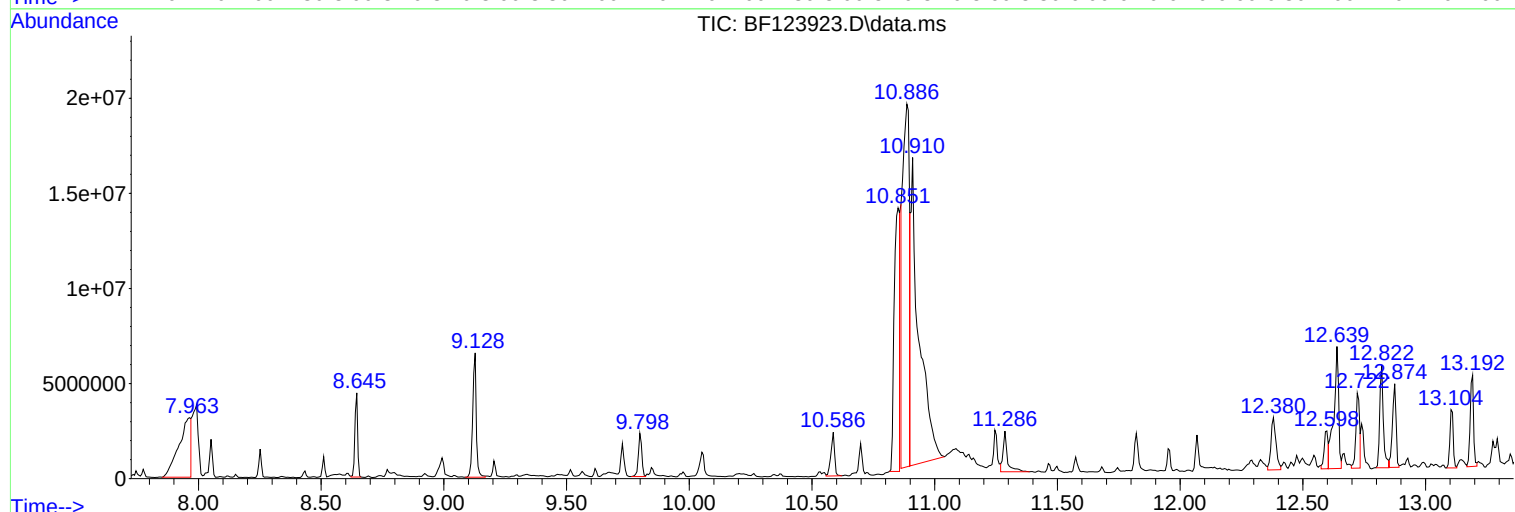
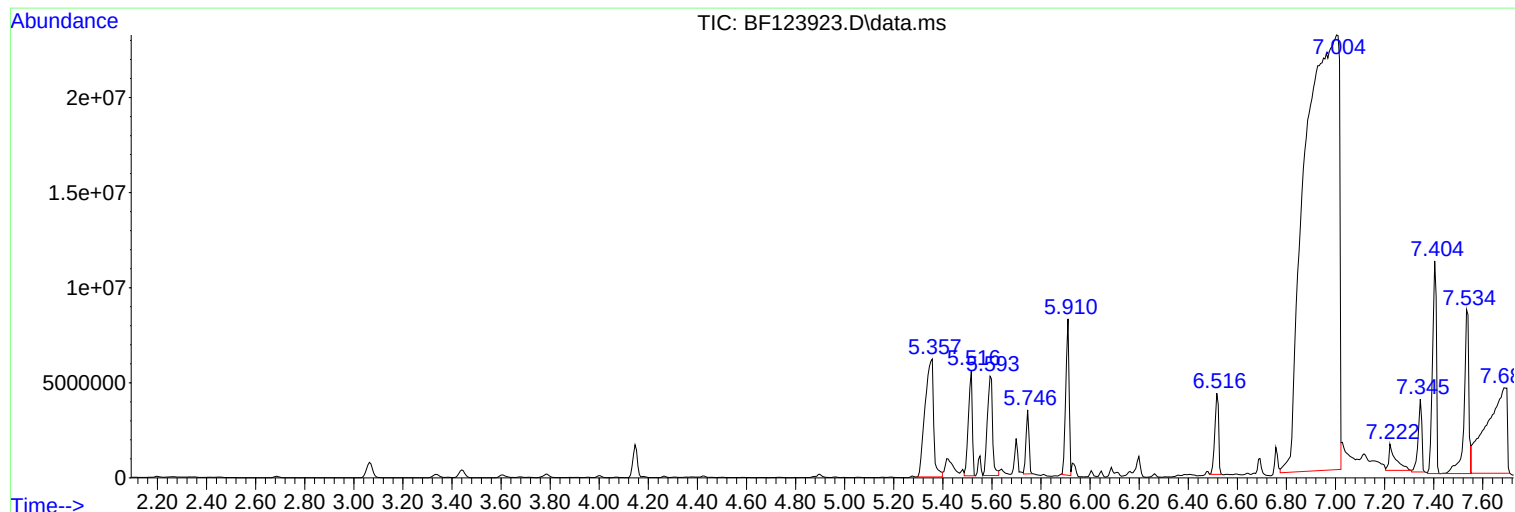
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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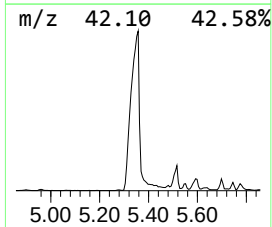
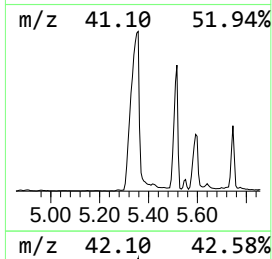
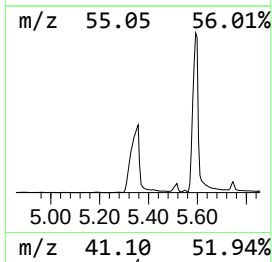
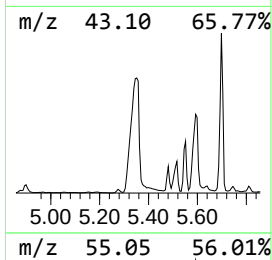
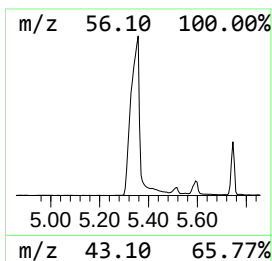
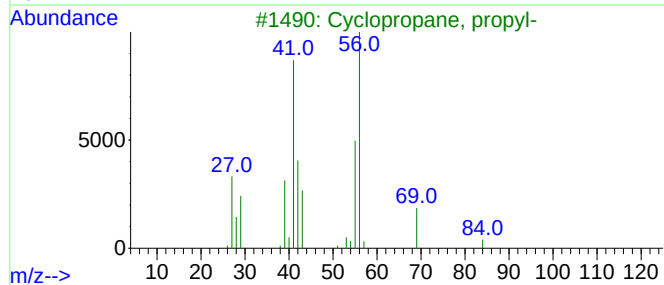
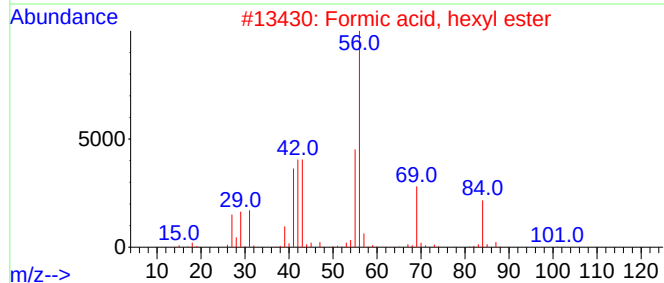
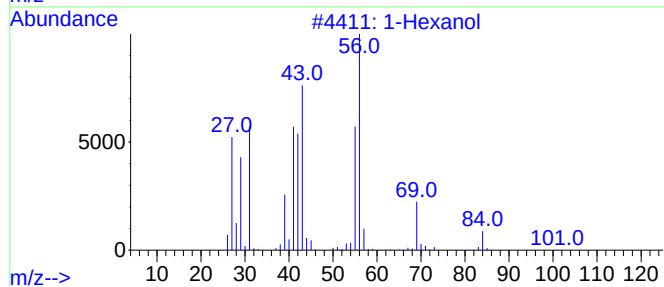
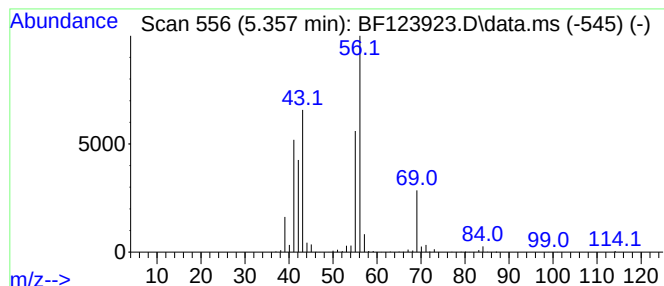
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Hexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.357	66.17 ng	15088000	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol			102	C6H14O	000111-27-3	83
2	Formic acid, hexyl ester			130	C7H14O2	000629-33-4	78
3	Cyclopropane, propyl-			84	C6H12	002415-72-7	64
4	1-Pentanol, 4-methyl-			102	C6H14O	000626-89-1	56
5	1-Butanol			74	C4H10O	000071-36-3	45



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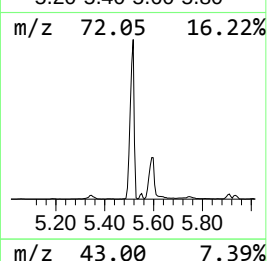
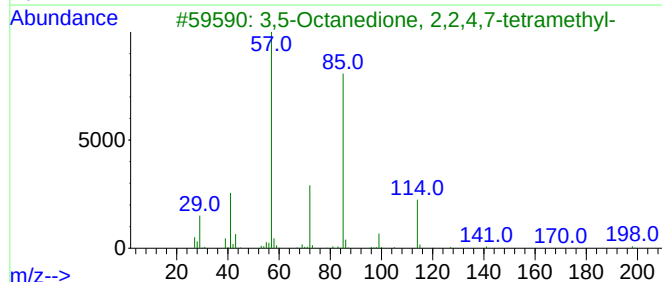
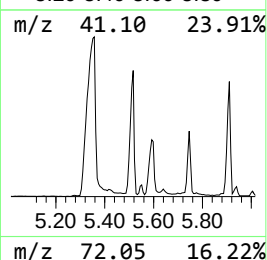
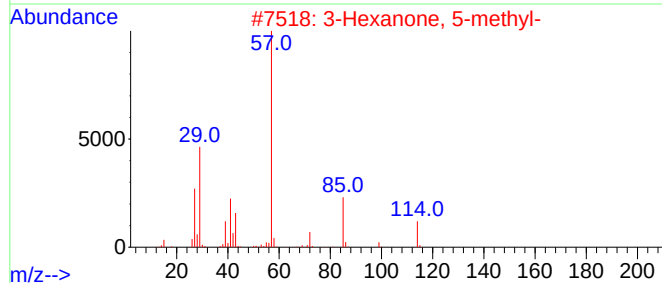
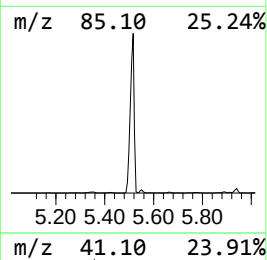
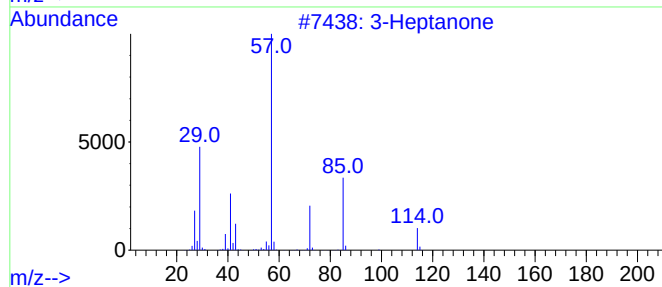
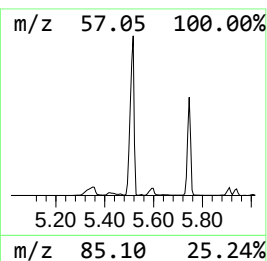
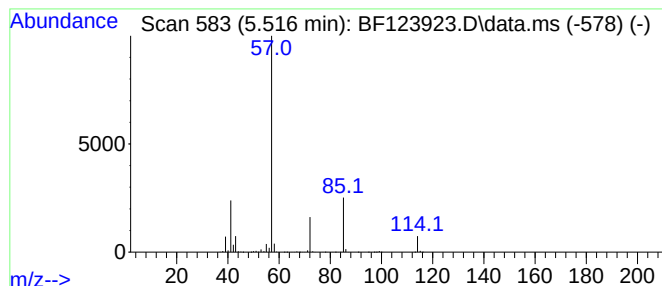
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Heptanone Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.516	26.55 ng	6053380	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone	114	C7H14O	000106-35-4	87
2			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	78
3			3,5-Octanedione, 2,2,4,7-tetrame...	198	C12H22O2	1000161-72-3	64
4			2,2-Dimethylpropanoic anhydride	186	C10H18O3	001538-75-6	40
5			2-Butanone, 1-bromo-3,3-dimethyl-	178	C6H11BrO	005469-26-1	38



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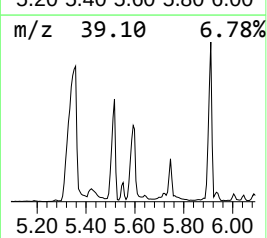
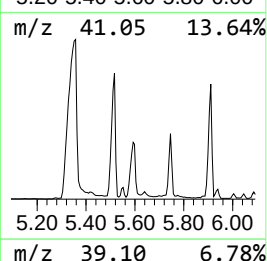
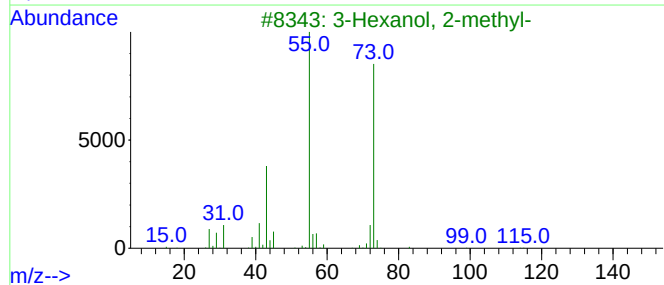
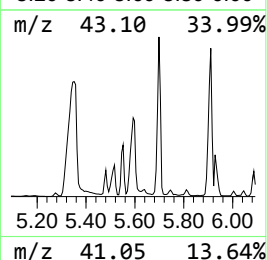
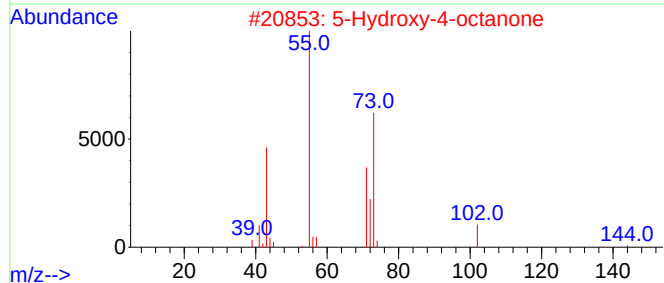
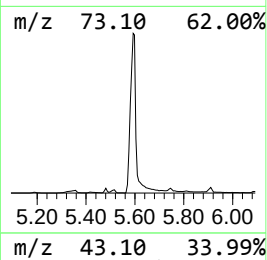
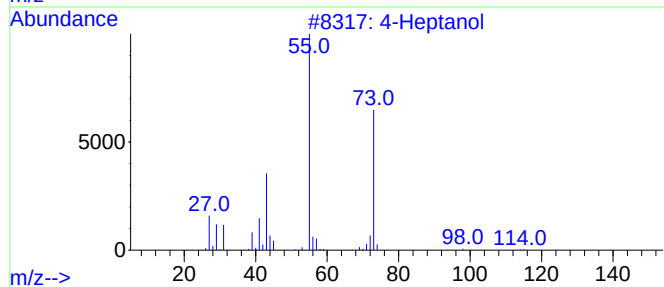
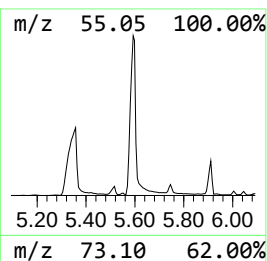
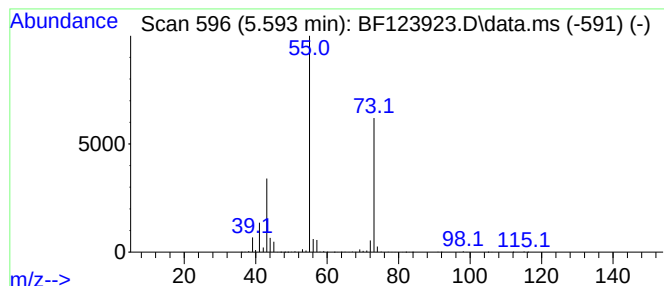
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Heptanol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.593	33.70 ng	7683960	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	83
2			5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	64
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	43
4			1-Hepten-4-ol	114	C7H14O	003521-91-3	39
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	27



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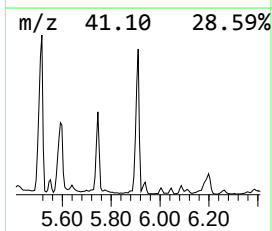
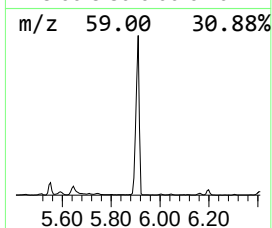
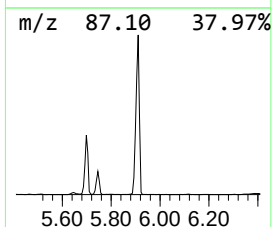
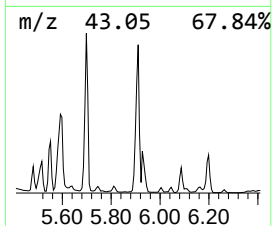
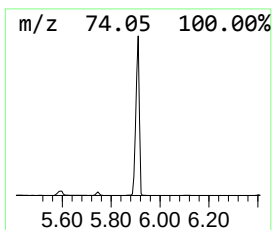
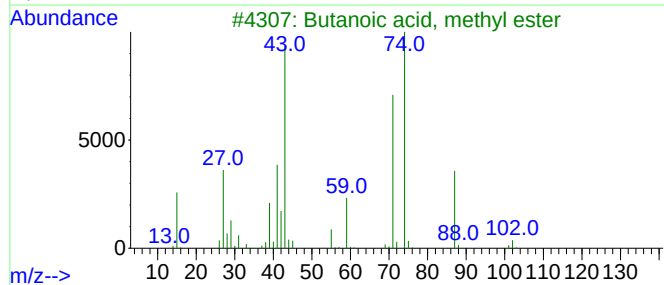
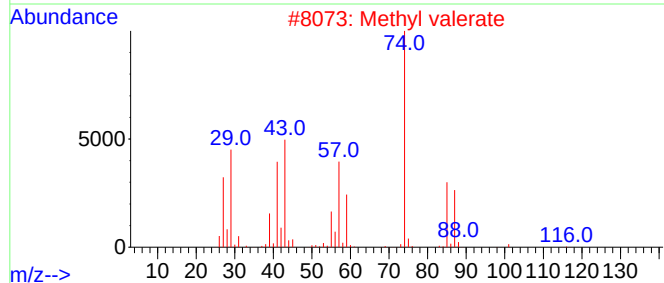
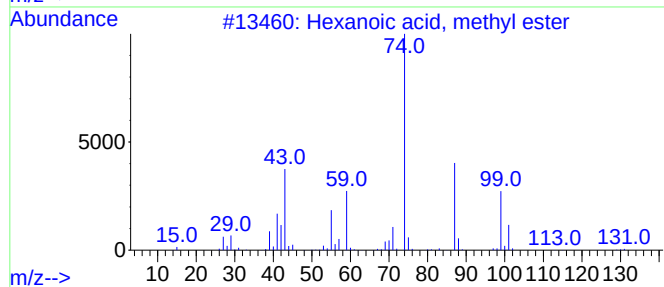
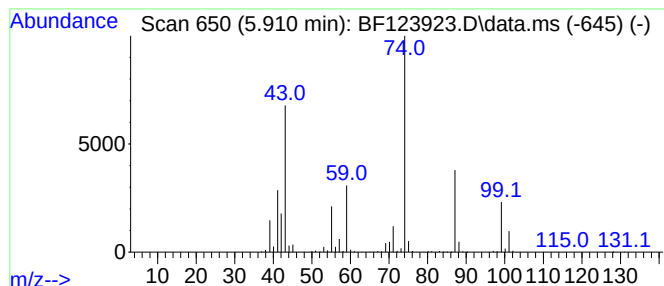
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanoic acid, methyl ester Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.910	34.38 ng	7838670	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	90
2			Methyl valerate	116	C6H12O2	000624-24-8	53
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	36
4			Tetramethylammonium tetrafluorob...	161	C4H12BF4N	000661-36-9	28
5			(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	10



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ClientSampleId :
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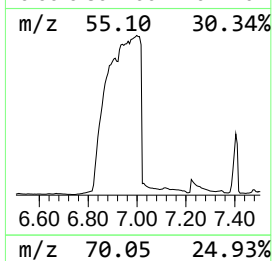
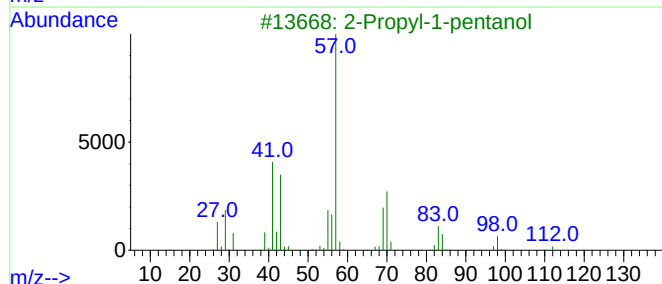
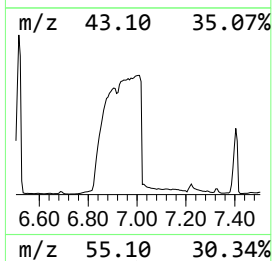
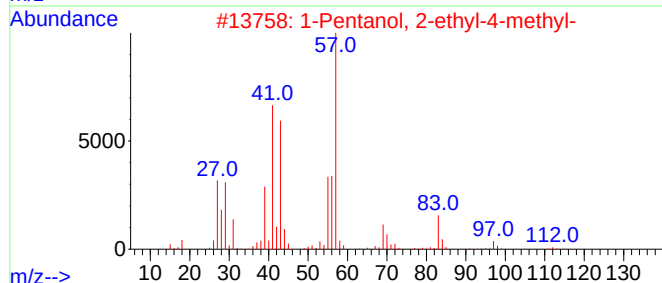
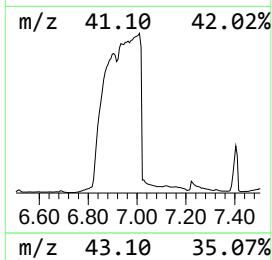
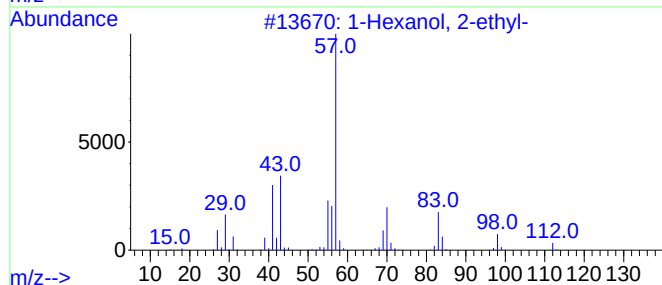
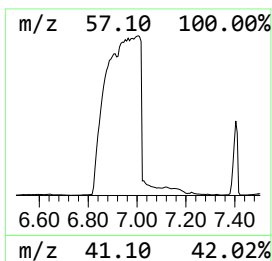
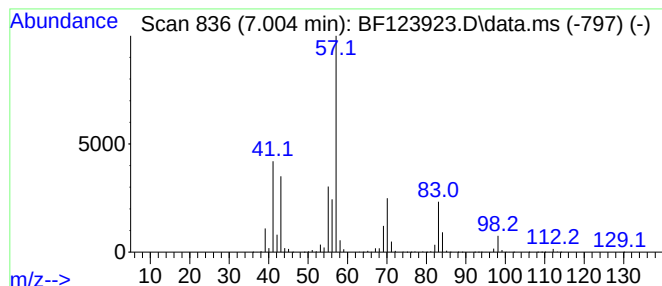
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.004	951.98 ng	217084000	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
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Instrument :
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ClientSampleId :
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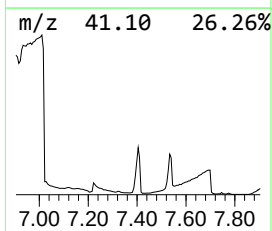
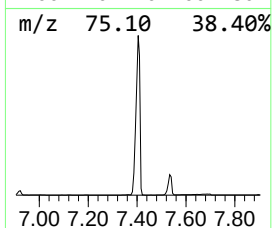
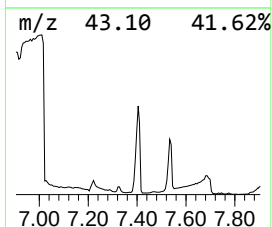
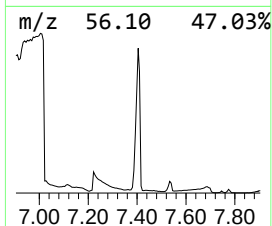
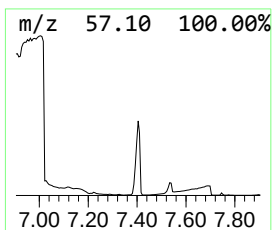
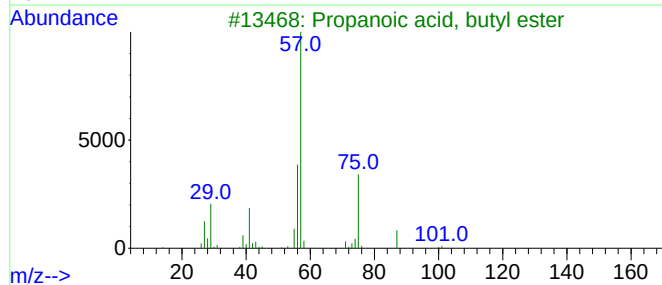
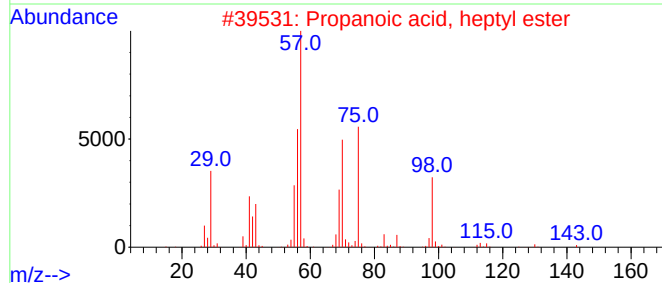
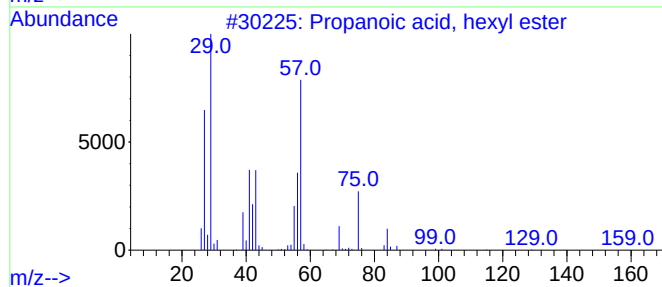
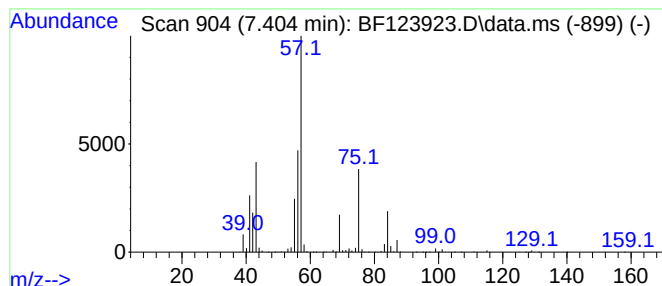
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Propanoic acid, hexyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.404	54.00 ng	12313100	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, hexyl ester	158	C9H18O2	002445-76-3	74
2			Propanoic acid, heptyl ester	172	C10H20O2	002216-81-1	45
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	45
4			Propanoic acid, octyl ester	186	C11H22O2	000142-60-9	40
5			Azetidine	57	C3H7N	000503-29-7	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
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Instrument :
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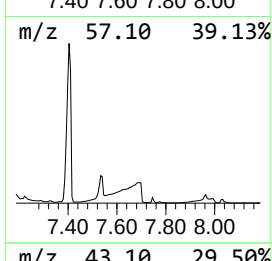
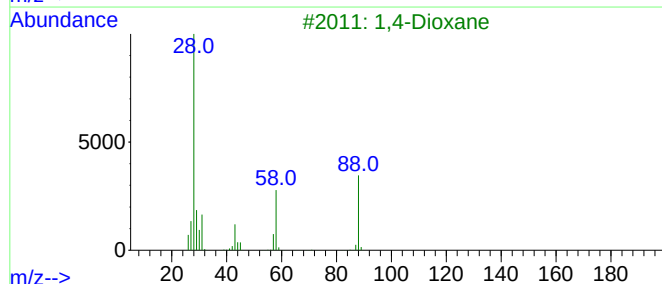
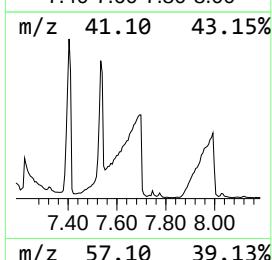
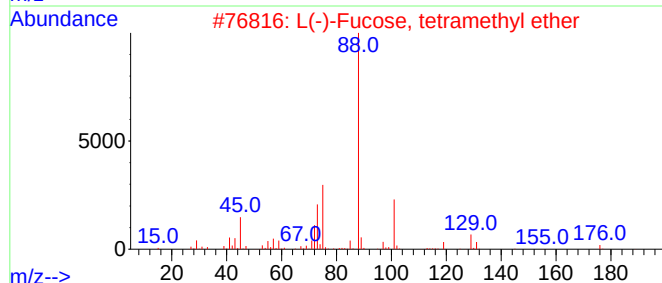
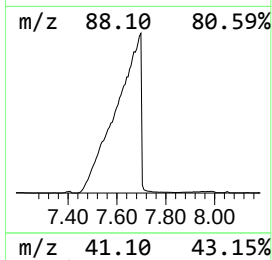
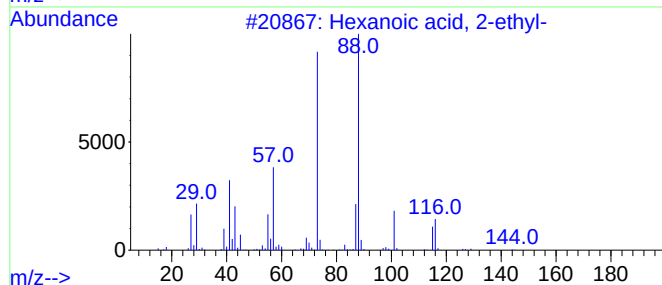
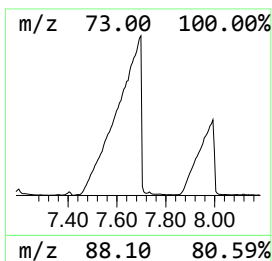
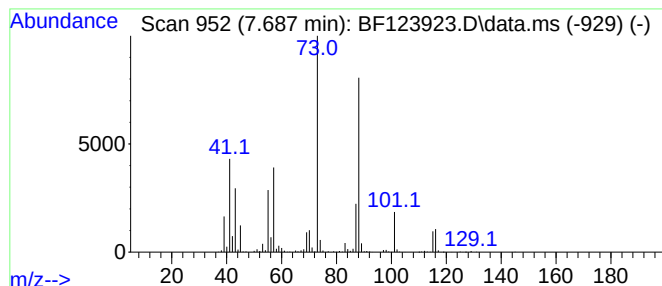
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	47.82 ng	25834200	Naphthalene-d8	8.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			L(-)-Fucose, tetramethyl ether	220	C10H20O5	1000332-75-0	43
3			1,4-Dioxane	88	C4H8O2	000123-91-1	43
4			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
5			Cyclohexanecarboxylic acid, .alpha.-...	170	C10H18O2	006051-00-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
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Sample : M2340-01
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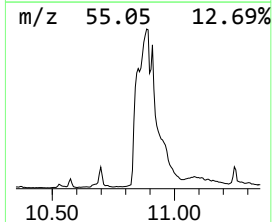
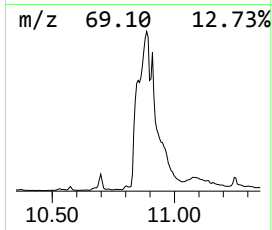
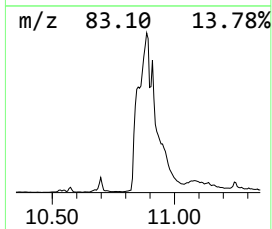
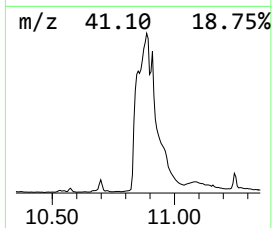
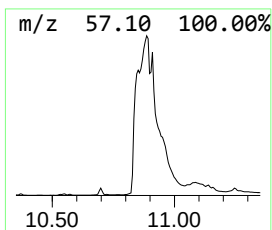
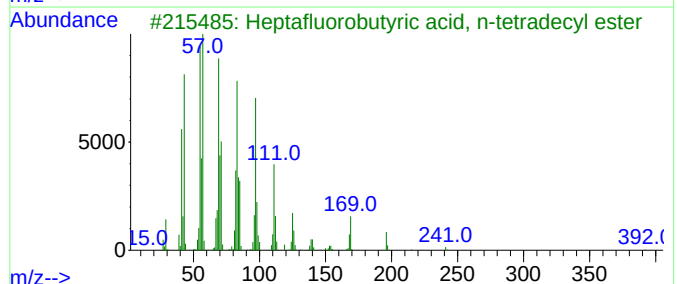
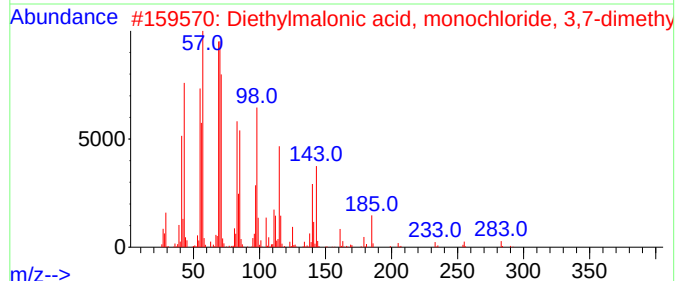
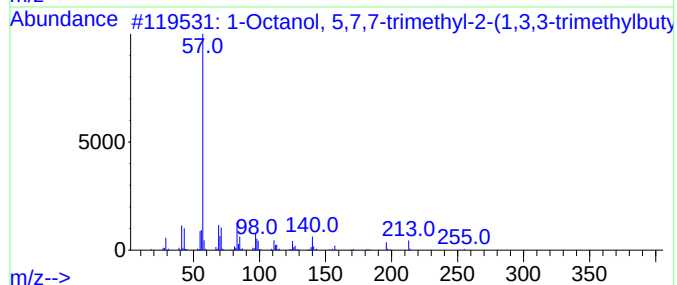
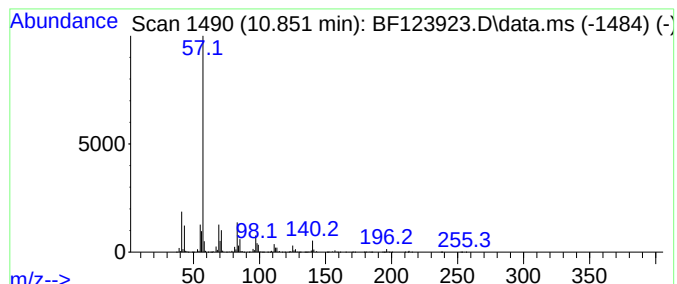
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	170.52 ng	22012800	Phenanthrene-d10	11.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	64	
2	Diethylmalonic acid, monochlorid...	318	C17H31ClO3	1000369-41-8	59	
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	59	
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	50	
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	50	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
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Sample : M2340-01
Misc :
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Instrument :
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ClientSampleId :
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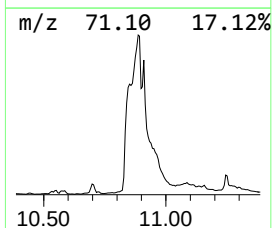
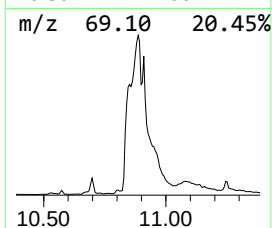
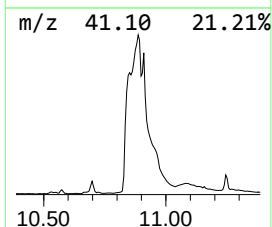
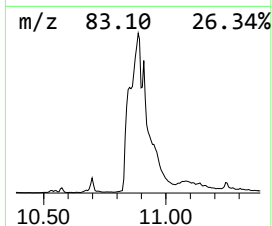
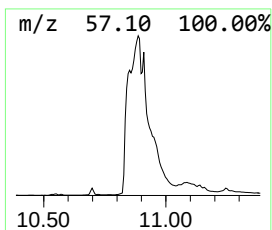
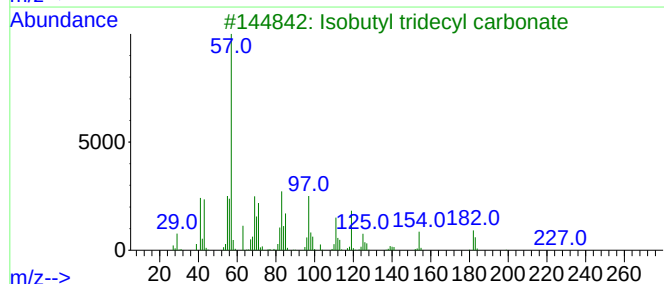
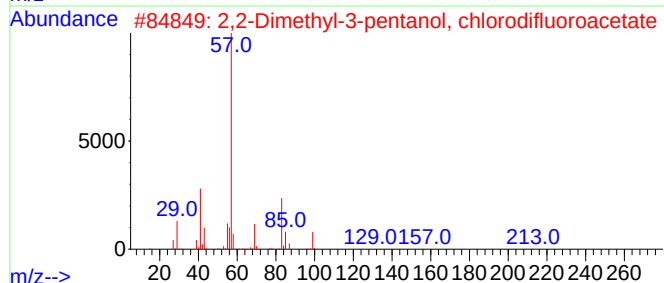
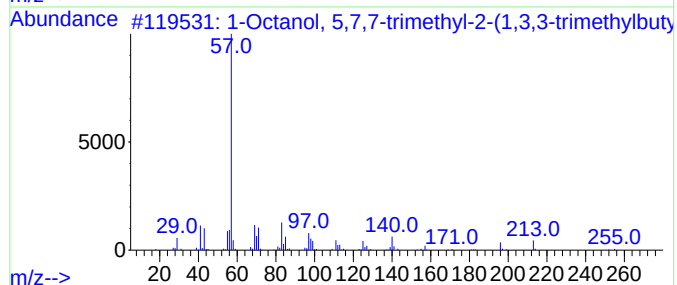
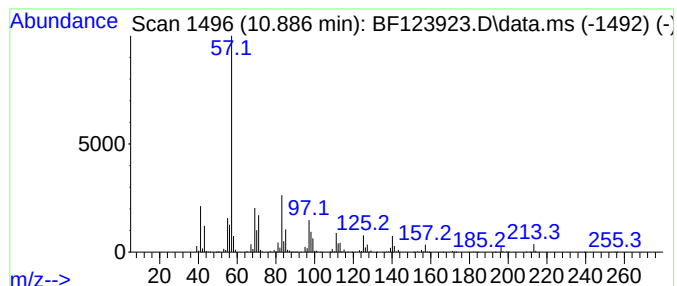
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown10.88 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.886	276.69 ng	35718500	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	64
2			2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	43
3			Isobutyl tridecyl carbonate	300	C18H36O3	959275-44-6	43
4			Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	38
5			Tridecane, 6-cyclohexyl-	266	C19H38	013151-91-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
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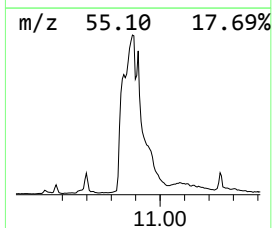
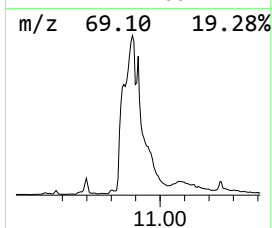
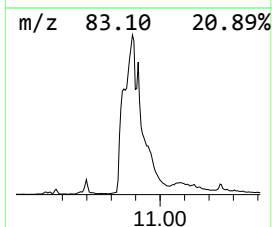
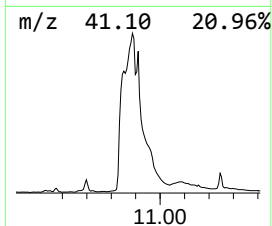
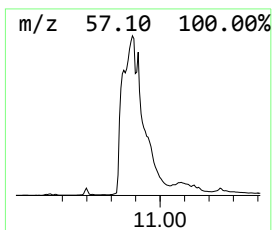
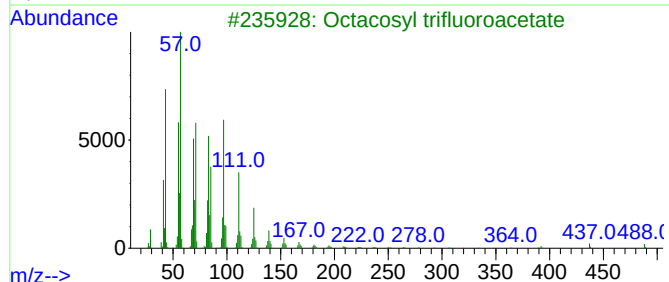
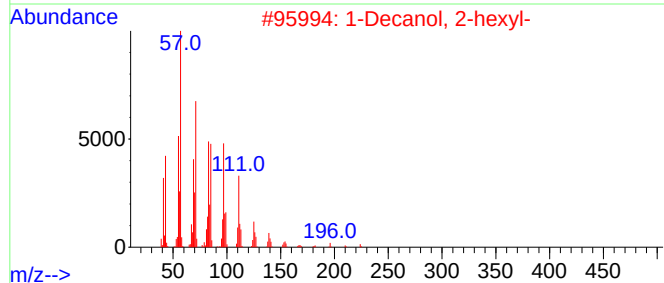
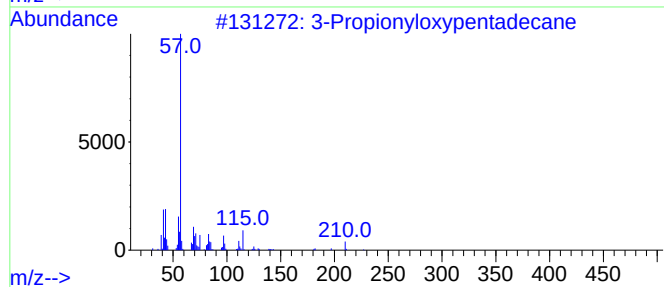
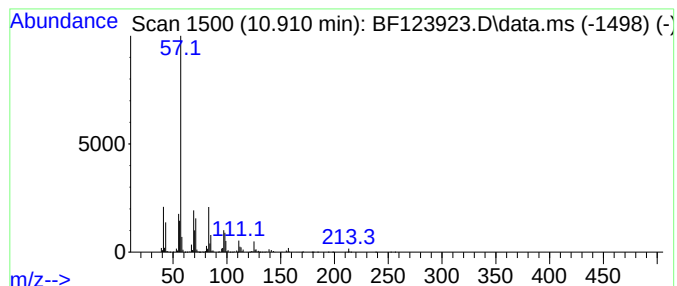
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 3-Propionyloxypentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.910	288.16 ng	37198600	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Propionyloxypentadecane	284	C18H36O2	1000245-63-1	53
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	50
3			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	50
4			Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	47
5			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
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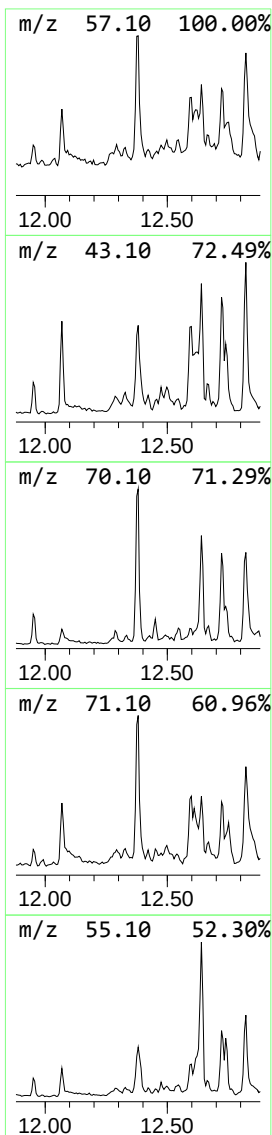
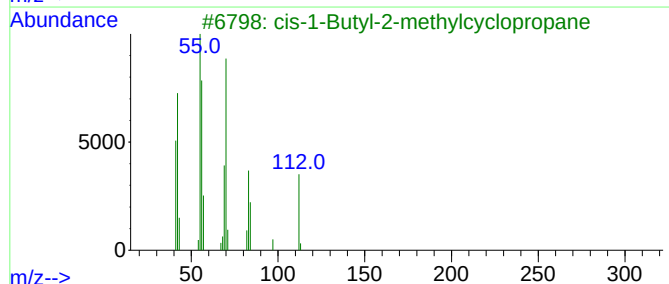
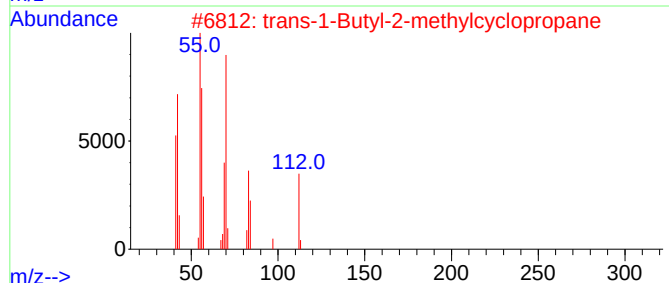
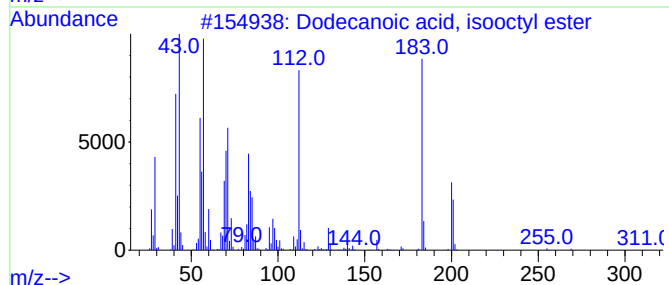
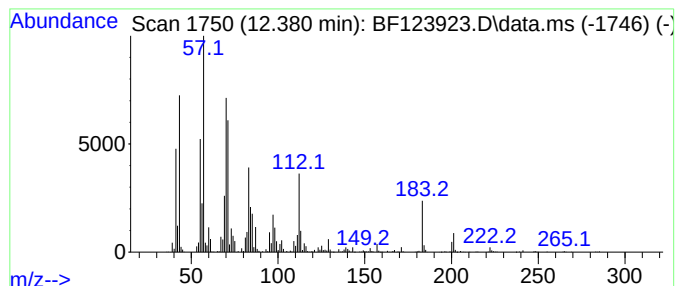
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Dodecanoic acid, isooctyl e... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.380	29.83 ng	3850890	Phenanthrene-d10	11.286	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, isooctyl ester	312	C20H40O2	084713-06-4	52
2	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	49
3	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	49
4	Formic acid, 2-ethylhexyl ester	158	C9H18O2	1000368-94-7	43
5	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
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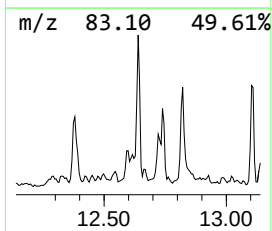
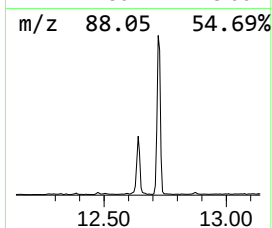
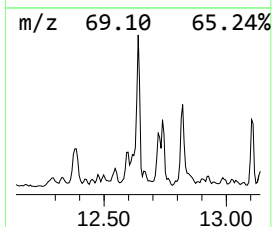
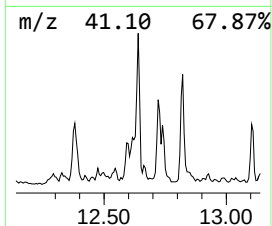
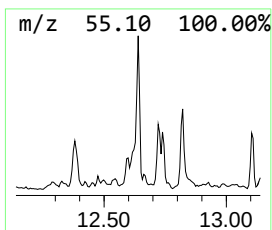
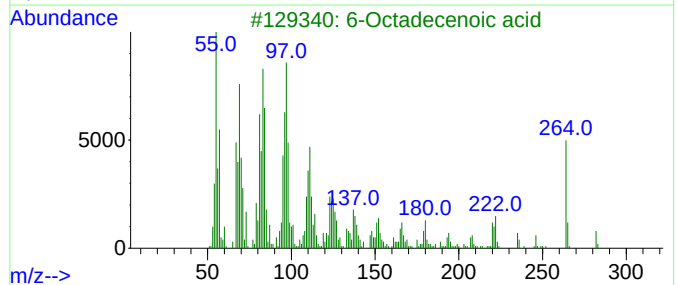
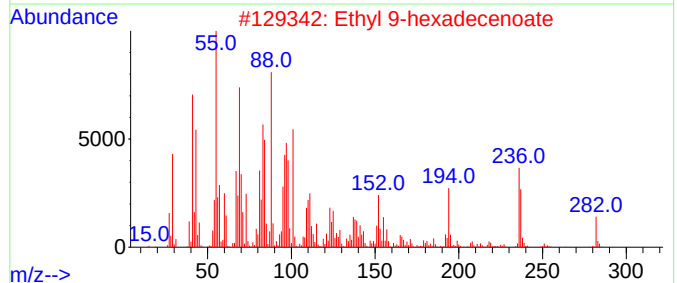
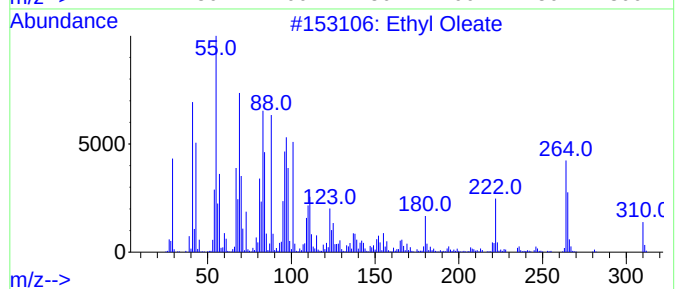
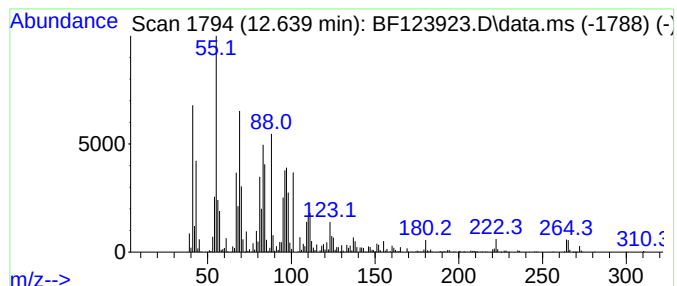
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Ethyl Oleate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	72.72 ng	8701350	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Oleate	310	C20H38O2	000111-62-6	94
2			Ethyl 9-hexadecenoate	282	C18H34O2	054546-22-4	91
3			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	68
4			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	62
5			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
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Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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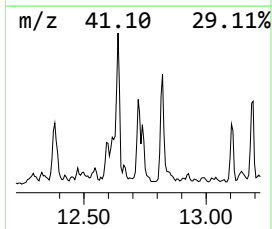
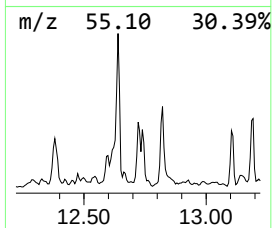
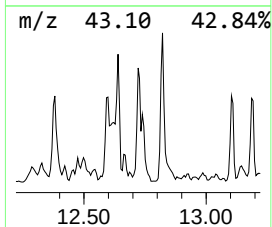
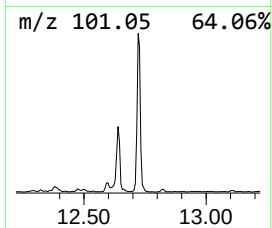
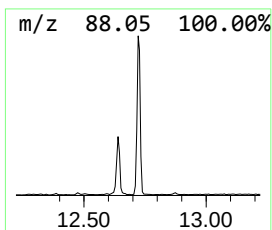
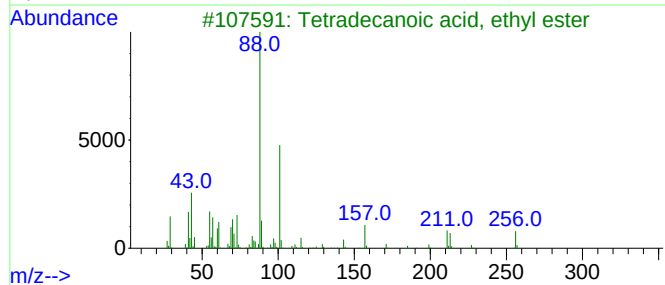
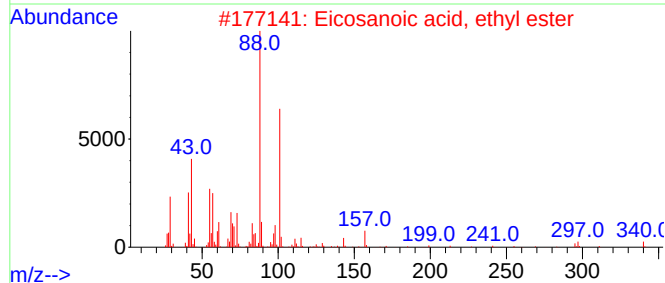
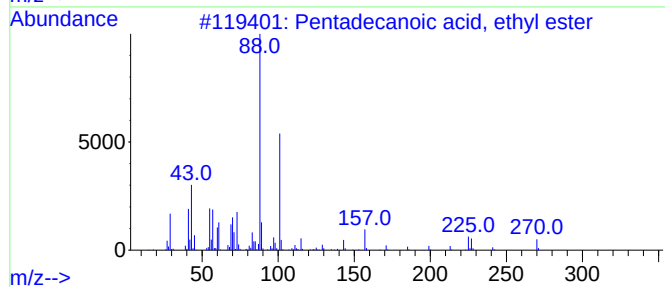
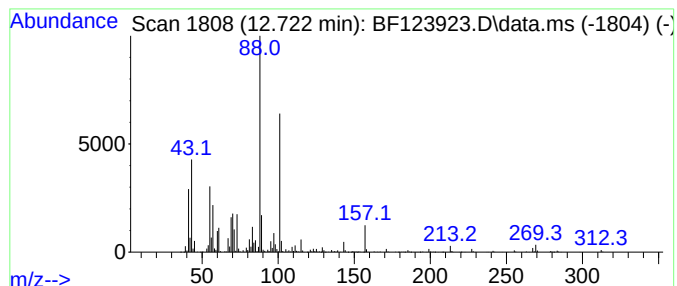
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Pentadecanoic acid, ethyl e... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	34.92 ng	4178310	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid, ethyl ester	270	C17H34O2	041114-00-5	91
2			Eicosanoic acid, ethyl ester	340	C22H44O2	018281-05-5	91
3			Tetradecanoic acid, ethyl ester	256	C16H32O2	000124-06-1	91
4			Hexadecanoic acid, ethyl ester	284	C18H36O2	000628-97-7	91
5			Heptadecanoic acid, ethyl ester	298	C19H38O2	014010-23-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

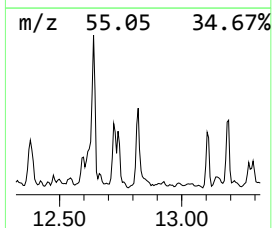
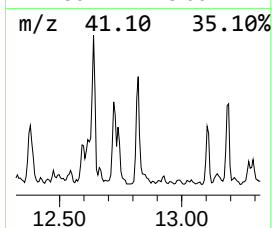
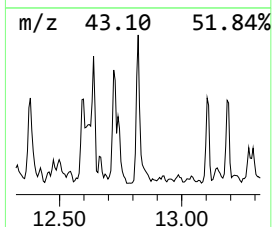
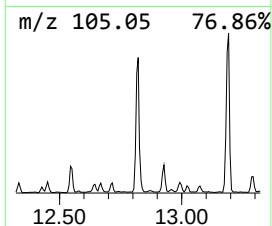
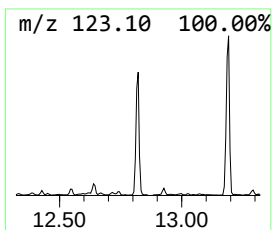
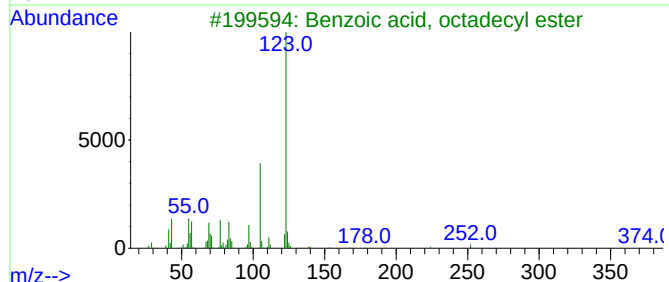
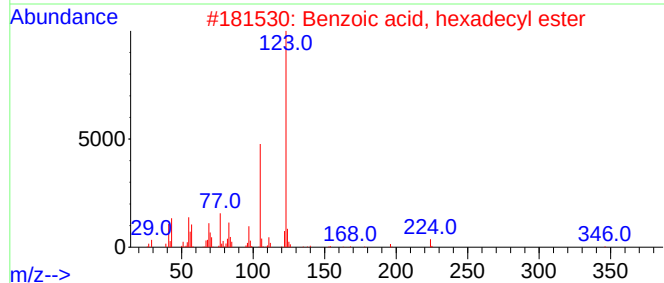
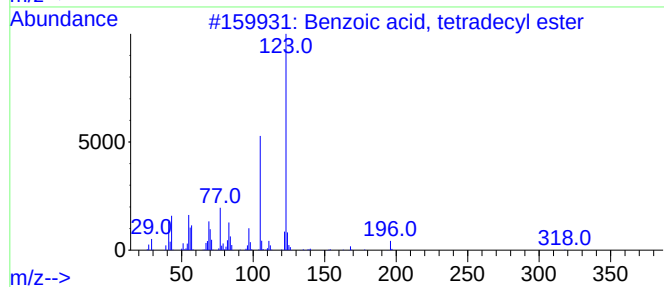
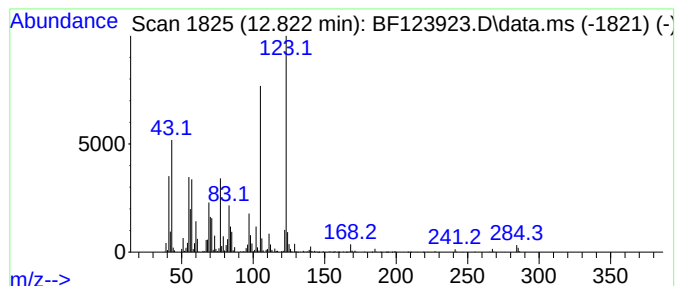
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Benzoic acid, tetradecyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
12.822	46.87 ng	5608610	Chrysene-d12		13.927		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	90
2			Benzoic acid, hexadecyl ester	346	C23H38O2	1000340-22-9	90
3			Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	83
4			Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	80
5			Benzoic acid, heptyl ester	220	C14H20O2	007155-12-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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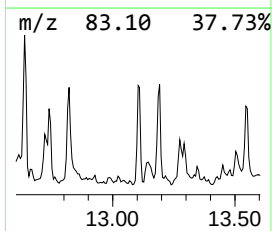
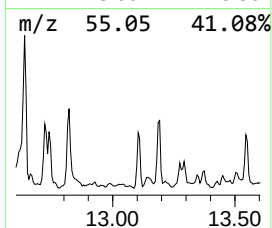
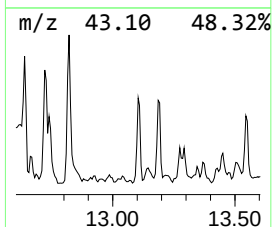
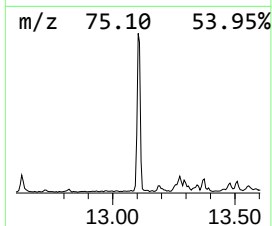
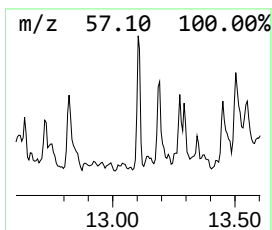
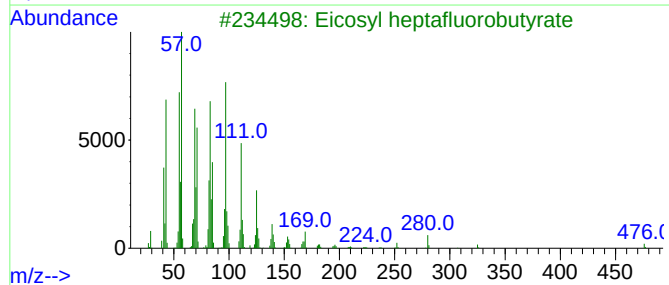
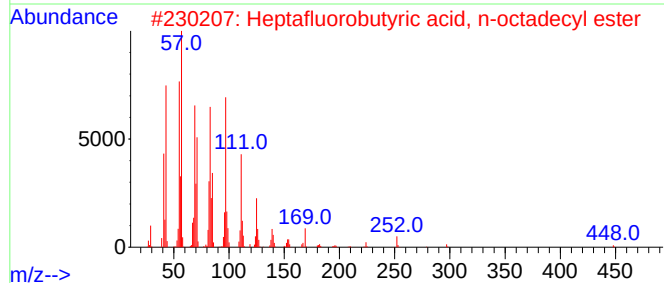
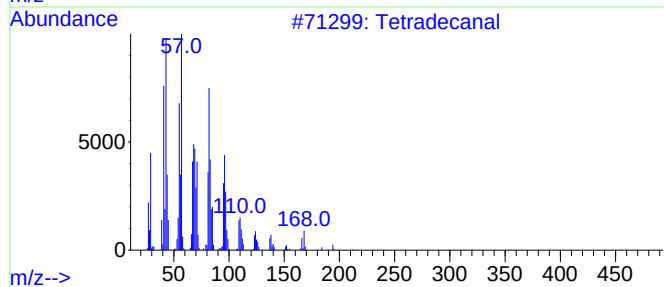
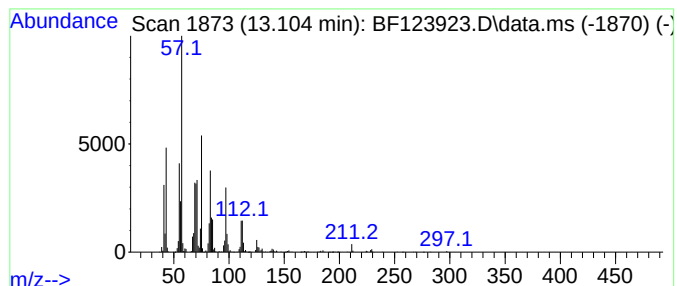
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Tetradecanal Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.104	24.19 ng	2893940	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanal	212	C14H28O	000124-25-4	53
2			Heptafluorobutyric acid, n-octadec...	466	C22H37F7O2	000400-57-7	49
3			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	47
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	47
5			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EFF-WW

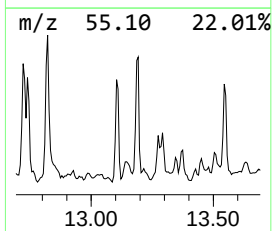
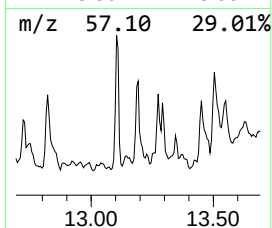
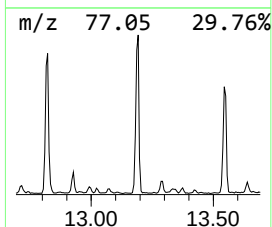
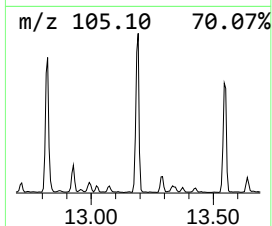
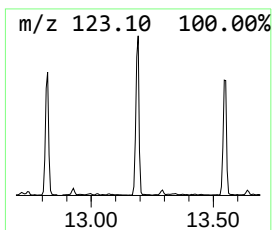
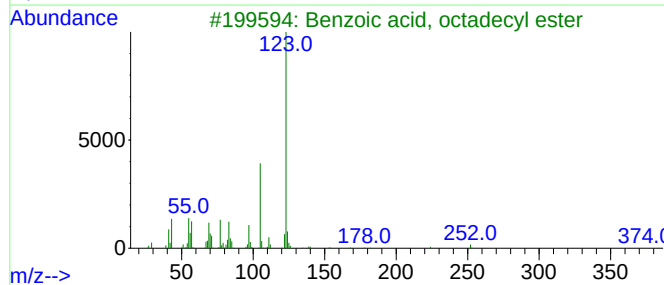
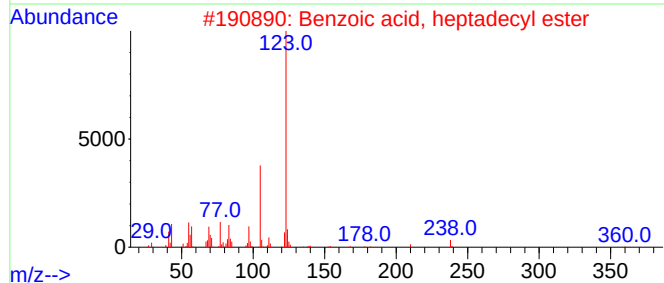
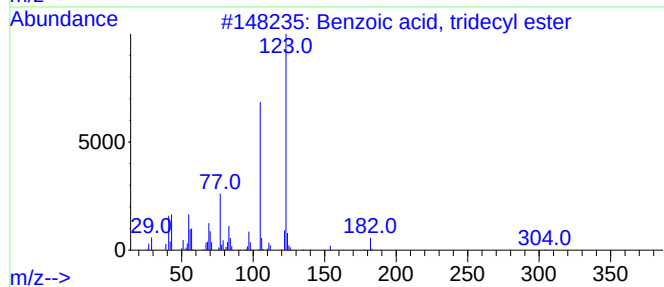
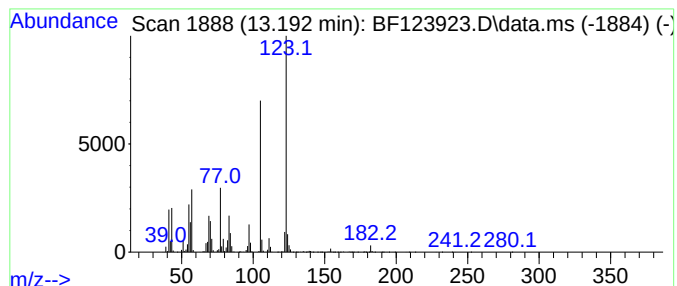
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Benzoic acid, tridecyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	38.16 ng	4566340	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	91
2			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	90
3			Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	90
4			Benzoic acid, eicosyl ester	402	C27H46O2	1000340-23-3	86
5			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EFF-WW

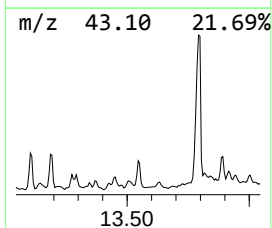
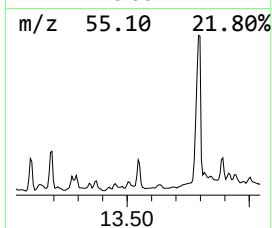
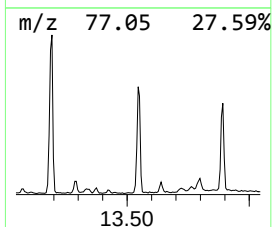
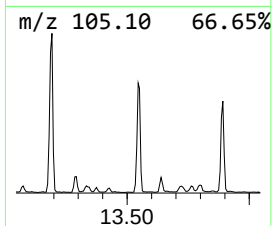
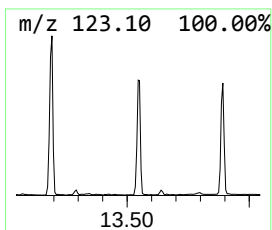
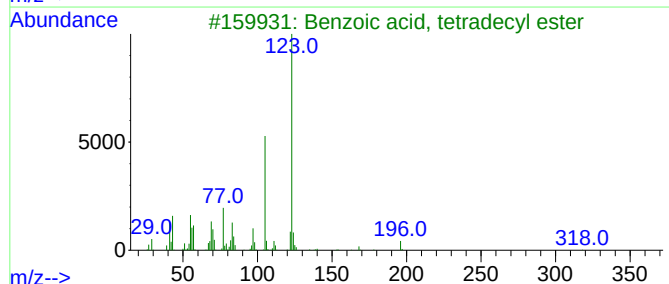
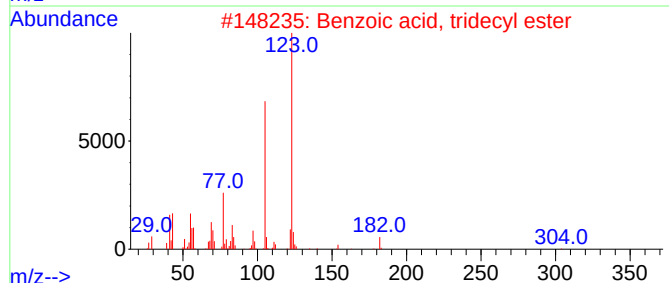
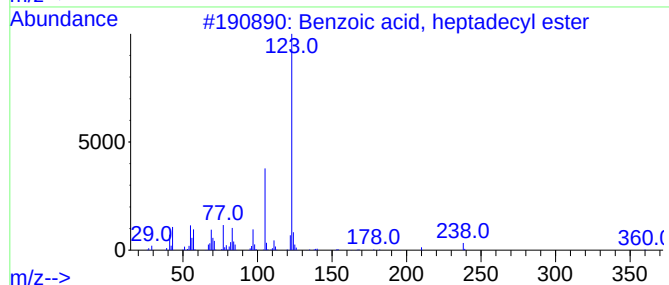
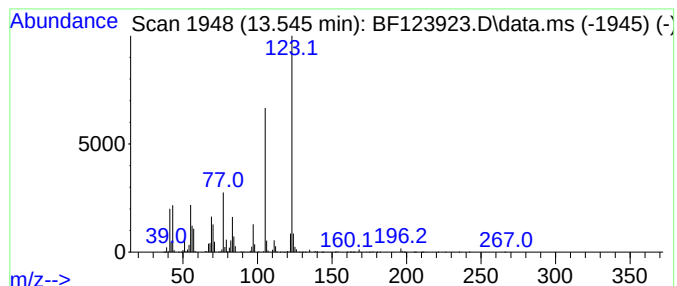
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Benzoic acid, heptadecyl ester Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.545	27.75 ng	3320290	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	91
2			Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	91
3			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	90
4			Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	90
5			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EFF-WW

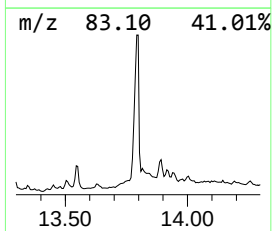
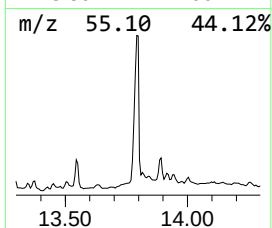
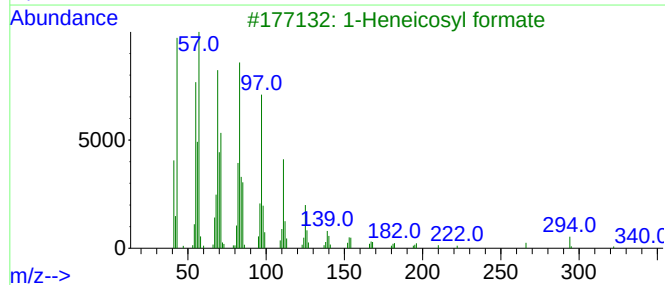
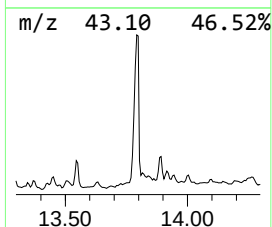
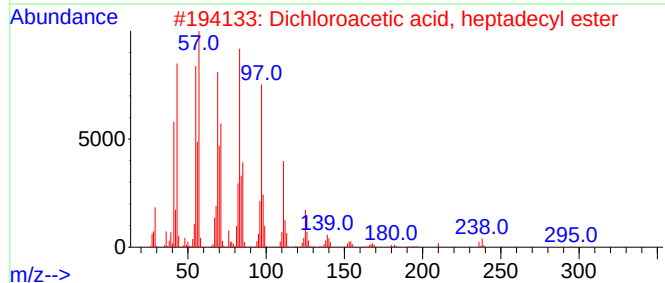
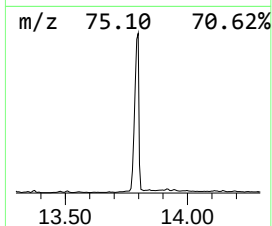
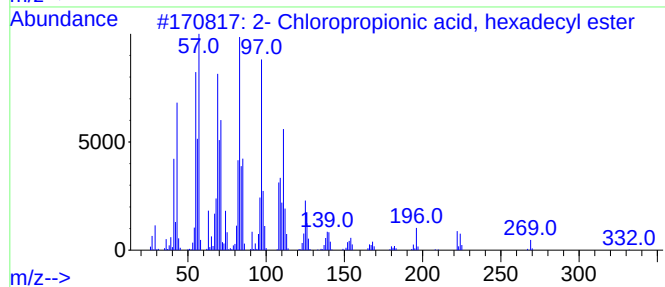
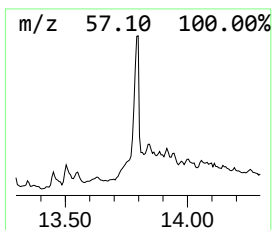
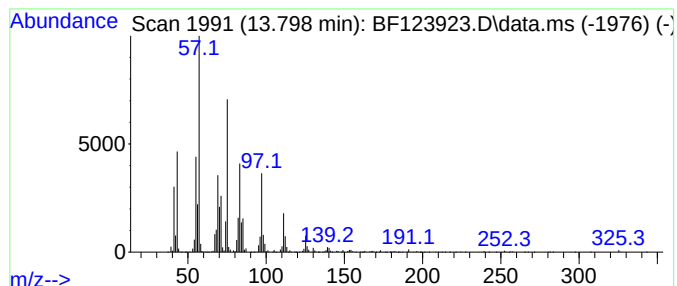
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 2- Chloropropionic acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	168.98 ng	20218900	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	70	
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	70		
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	70		
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	68		
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	68		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
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Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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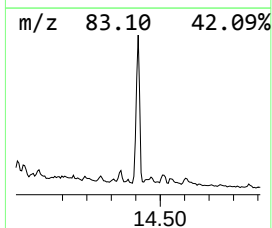
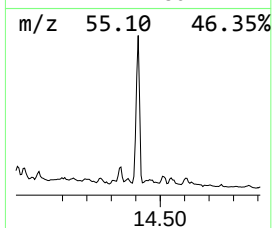
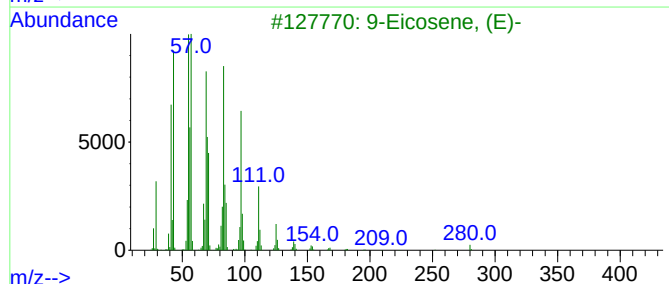
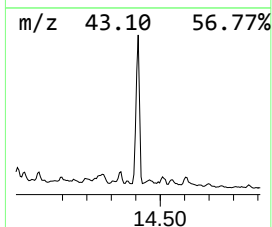
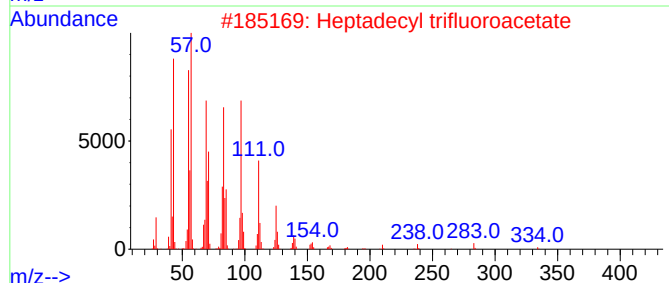
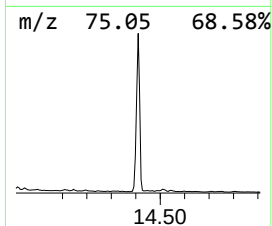
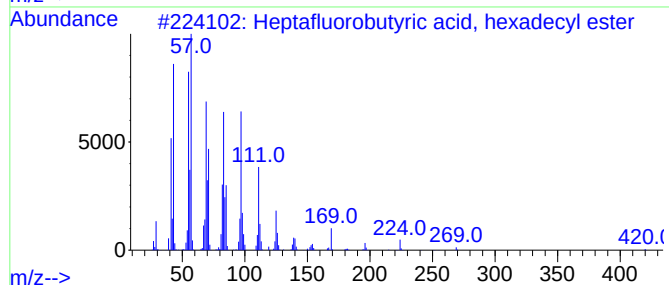
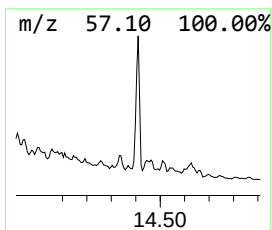
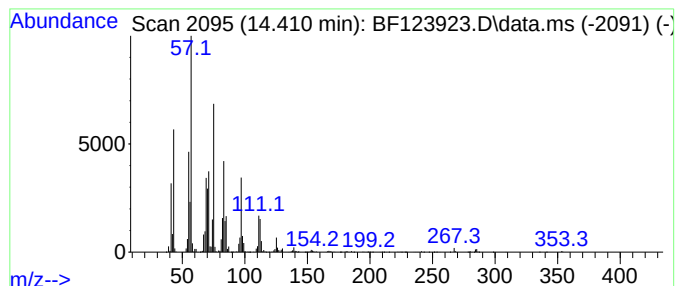
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Heptafluorobutyric acid, he... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.410	83.16 ng	9950520	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	58
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	58
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	58
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051221\
Data File : BF123923.D
Acq On : 12 May 2021 14:36
Operator : JU/CG
Sample : M2340-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

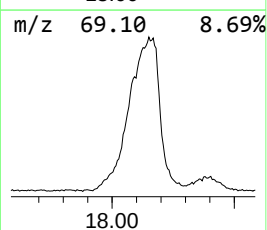
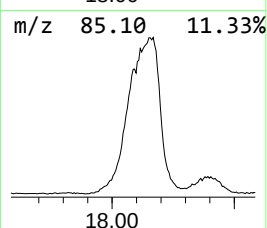
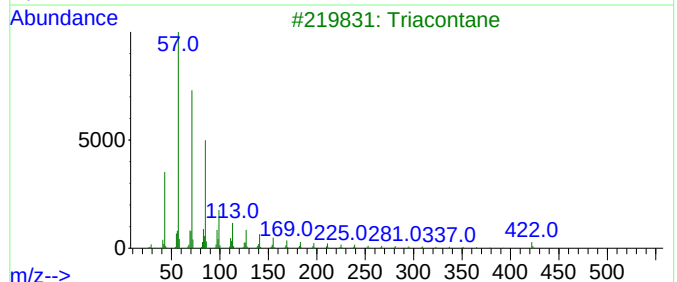
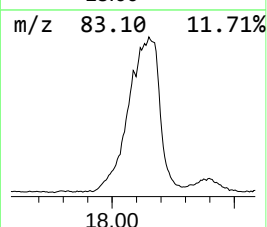
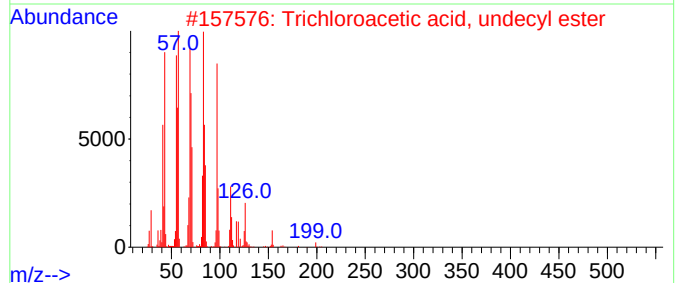
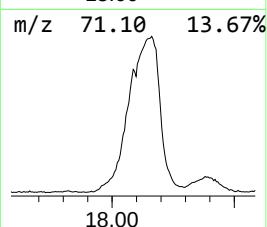
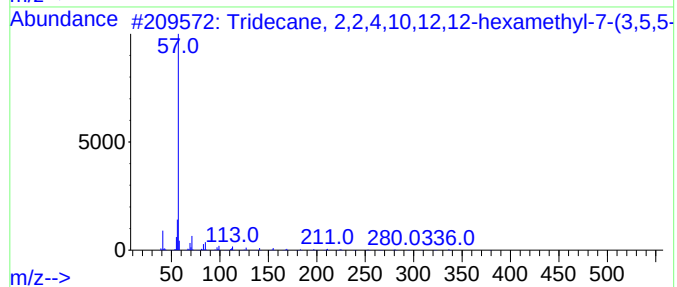
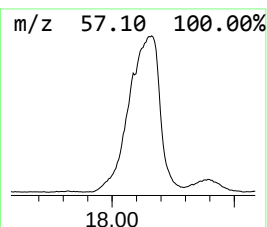
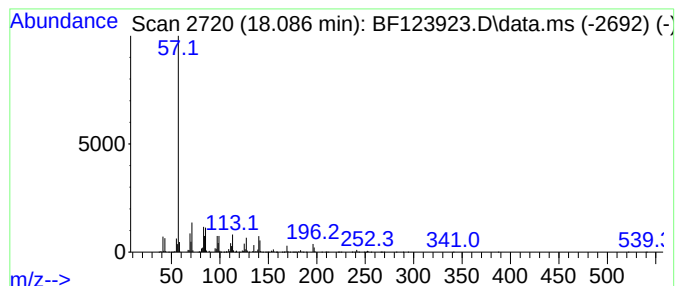
Instrument :
BNA_F
ClientSampleId :
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Tridecane, 2,2,4,10,12,12-h... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.086	41.16 ng	24634500	Perylene-d12	15.368	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2,2,4,10,12,12-hexame...	394	C28H58	003035-75-4	50
2	Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	50
3	Triacontane	422	C30H62	000638-68-6	43
4	Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	43
5	2,2,4,4,5,5,7,7-Octamethyloctane	226	C16H34	005171-85-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF0511221\
 Data File : BF123923.D
 Acq On : 12 May 2021 14:36
 Operator : JU/CG
 Sample : M2340-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol	5.357	66.2	ng	15088000	1	6.757	4560670	20.0
3-Heptanone	5.516	26.6	ng	6053380	1	6.757	4560670	20.0
4-Heptanol	5.593	33.7	ng	7683960	1	6.757	4560670	20.0
Hexanoic acid, ...	5.910	34.4	ng	7838670	1	6.757	4560670	20.0
1-Hexanol, 2-et...	7.004	952.0	ng	217084000	1	6.757	4560670	20.0
Propanoic acid,...	7.404	54.0	ng	12313100	1	6.757	4560670	20.0
Hexanoic acid, ...	7.687	47.8	ng	25834200	2	8.051	10804600	20.0
1-Octanol, 5,7,...	10.851	170.5	ng	22012800	4	11.286	2581810	20.0
unknown10.88	10.886	276.7	ng	35718500	4	11.286	2581810	20.0
3-Propionyloxyp...	10.910	288.2	ng	37198600	4	11.286	2581810	20.0
Dodecanoic acid...	12.380	29.8	ng	3850890	4	11.286	2581810	20.0
Ethyl Oleate	12.639	72.7	ng	8701350	5	13.927	2393110	20.0
Pentadecanoic a...	12.722	34.9	ng	4178310	5	13.927	2393110	20.0
Benzoic acid, t...	12.822	46.9	ng	5608610	5	13.927	2393110	20.0
Tetradecanal	13.104	24.2	ng	2893940	5	13.927	2393110	20.0
Benzoic acid, t...	13.192	38.2	ng	4566340	5	13.927	2393110	20.0
Benzoic acid, h...	13.545	27.8	ng	3320290	5	13.927	2393110	20.0
2-Chloropropio...	13.798	169.0	ng	20218900	5	13.927	2393110	20.0
Heptafluorobuty...	14.410	83.2	ng	9950520	5	13.927	2393110	20.0
Tridecane, 2,2,...	18.086	41.2	ng	24634500	6	15.368	11969800	20.0