

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
 Data File : BF131050.D
 Acq On : 07 Nov 2022 18:54
 Operator : CG\JU
 Sample : N5415-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R-16

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-BF110722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131050.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	11	18	25	rBV	652126	782003	34.10%	4.731%
2	2.305	32	37	42	rBV	41068	53506	2.33%	0.324%
3	4.504	407	411	416	rBV	62959	68348	2.98%	0.413%
4	5.128	512	517	529	rVB	400387	490807	21.40%	2.969%
5	5.522	579	584	587	rBV	2025618	1937949	84.51%	11.724%
6	6.528	749	755	758	rBV	2043399	2122705	92.57%	12.842%
7	6.898	814	818	821	rBV	716881	533289	23.26%	3.226%
8	7.463	909	914	917	rBV	1283307	1211516	52.83%	7.329%
9	8.181	1032	1036	1040	rBV	734042	664810	28.99%	4.022%
10	9.263	1214	1220	1223	rBV	2818794	2293170	100.00%	13.873%
11	9.945	1332	1336	1339	rBV	888998	773591	33.73%	4.680%
12	10.733	1466	1470	1473	rBV	1575445	1303815	56.86%	7.888%
13	11.433	1585	1589	1592	rBV	897968	749059	32.66%	4.532%
14	11.951	1672	1677	1682	rBV5	20188	30138	1.31%	0.182%
15	12.651	1792	1796	1799	rVB	57588	43186	1.88%	0.261%
16	12.880	1829	1835	1838	rBV	58944	65773	2.87%	0.398%
17	13.021	1855	1859	1863	rBV	1666591	1532284	66.82%	9.270%
18	13.921	2009	2012	2014	rBV2	37066	32276	1.41%	0.195%
19	13.957	2014	2018	2031	rVB3	65670	167116	7.29%	1.011%
20	14.080	2032	2039	2042	rBV	597157	562580	24.53%	3.403%
21	14.180	2052	2056	2060	rVB	34135	40765	1.78%	0.247%
22	14.233	2062	2065	2069	rBV	31988	36409	1.59%	0.220%
23	14.539	2115	2117	2121	rBV	45362	45415	1.98%	0.275%
24	14.598	2123	2127	2138	rVV7	40788	102762	4.48%	0.622%
25	14.857	2168	2171	2176	rVB3	29399	38164	1.66%	0.231%
26	15.139	2215	2219	2222	rBV	36440	52333	2.28%	0.317%
27	15.210	2227	2231	2235	rVB	50655	57949	2.53%	0.351%
28	15.515	2280	2283	2289	rVB	39504	62891	2.74%	0.380%
29	15.580	2289	2294	2301	rBV	348323	460535	20.08%	2.786%
30	16.051	2372	2374	2379	rVB3	21022	30687	1.34%	0.186%
31	16.580	2461	2464	2468	rBV5	25631	38767	1.69%	0.235%
32	16.751	2490	2493	2497	rBV5	22203	32778	1.43%	0.198%
33	16.892	2513	2517	2524	rVB9	22417	44892	1.96%	0.272%
34	17.504	2619	2621	2624	rBV4	20873	34805	1.52%	0.211%
35	17.780	2666	2668	2677	rVB9	16068	32824	1.43%	0.199%

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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-BF110722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

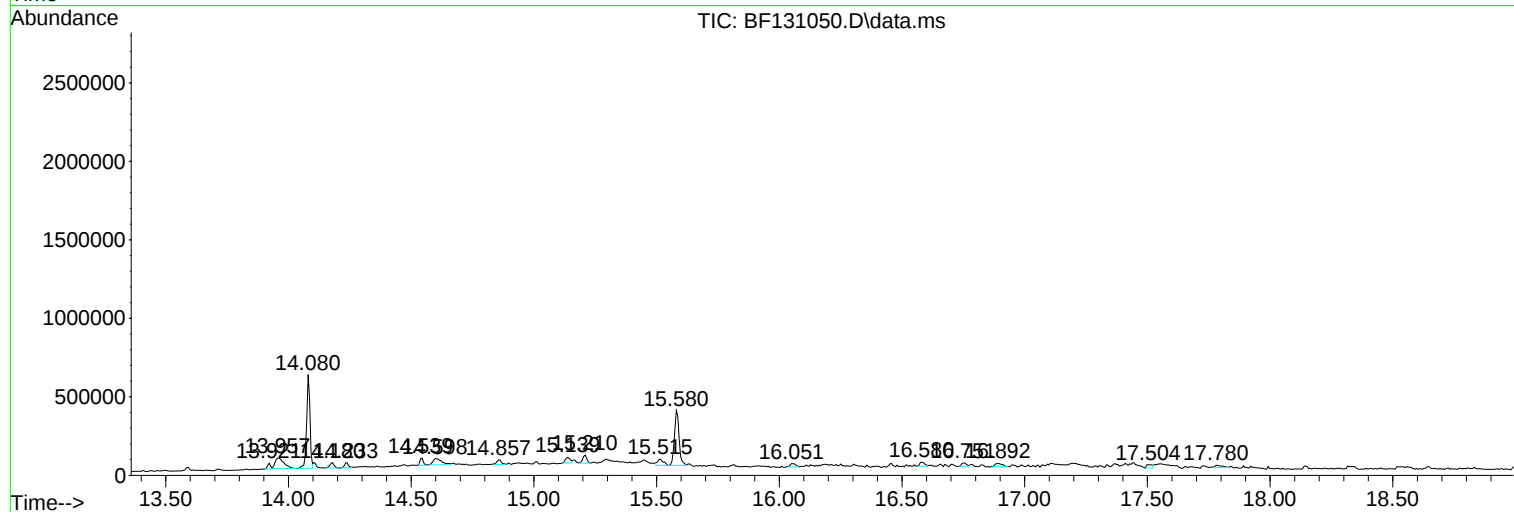
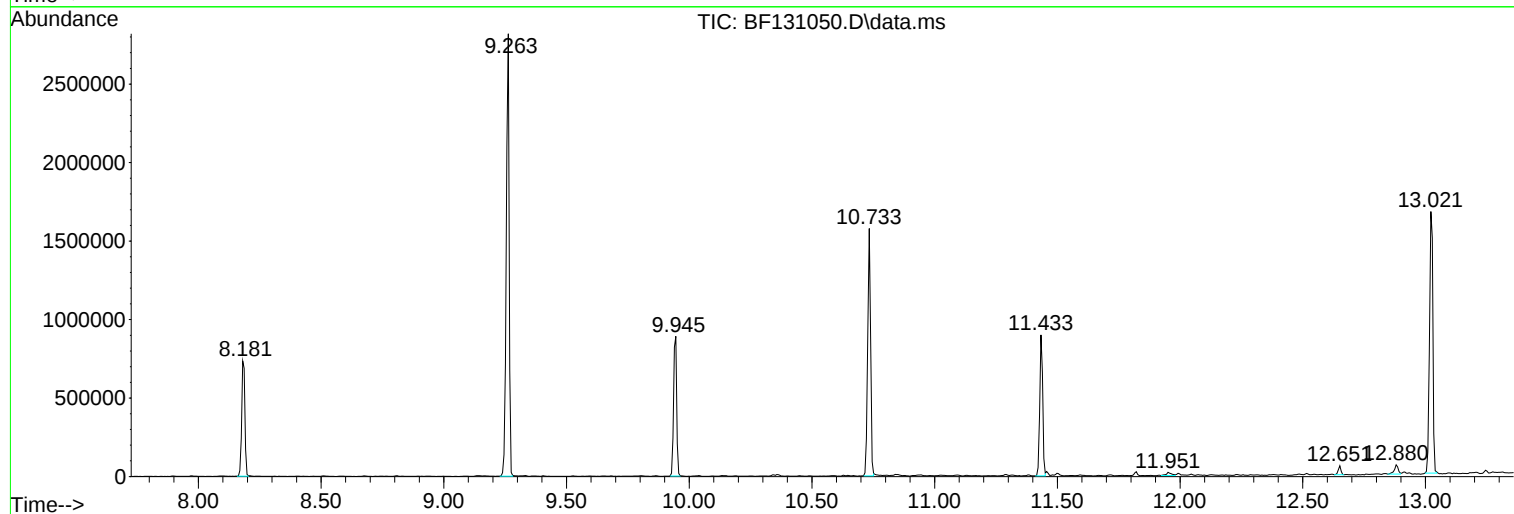
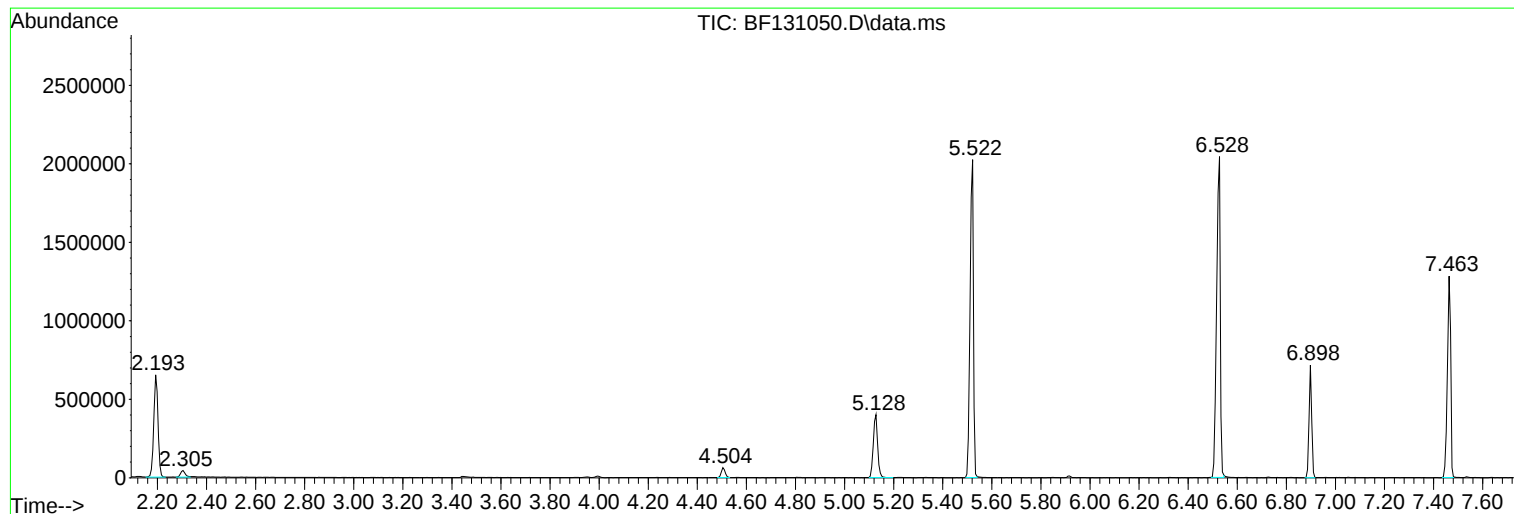
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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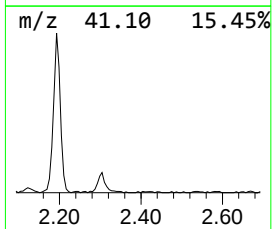
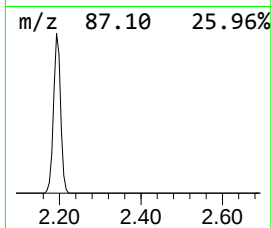
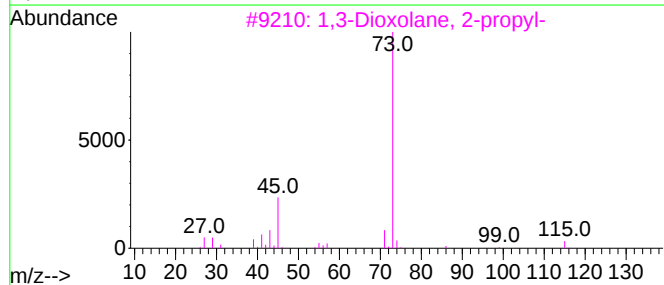
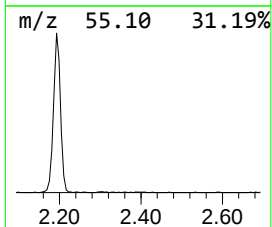
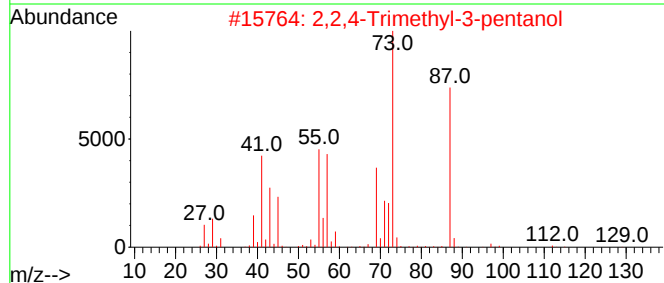
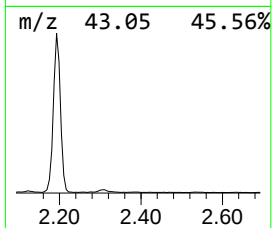
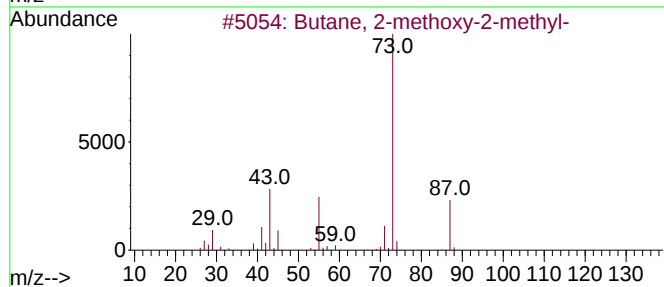
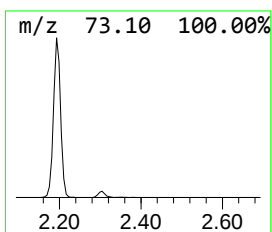
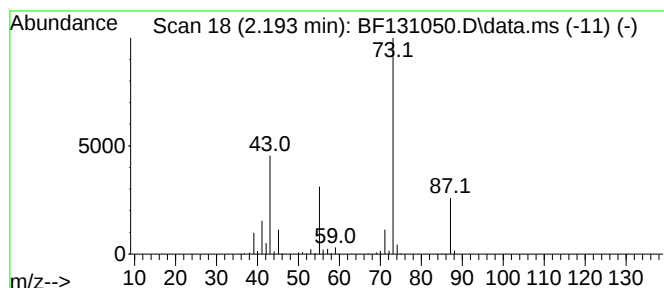
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	29.33 ng	782003	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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Instrument :
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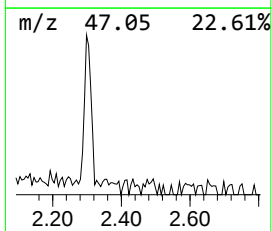
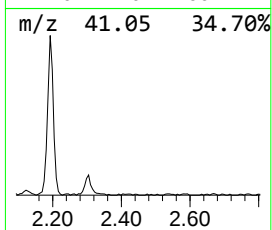
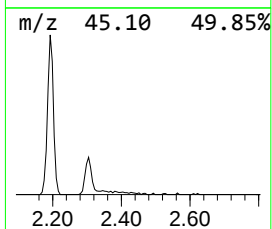
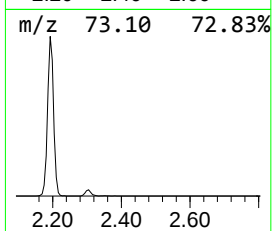
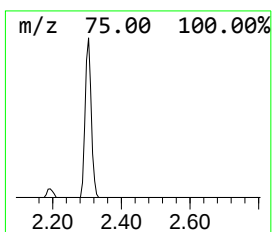
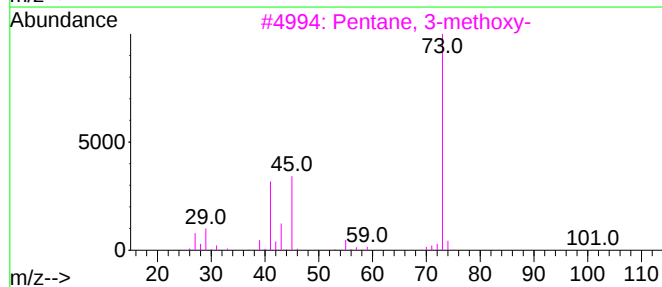
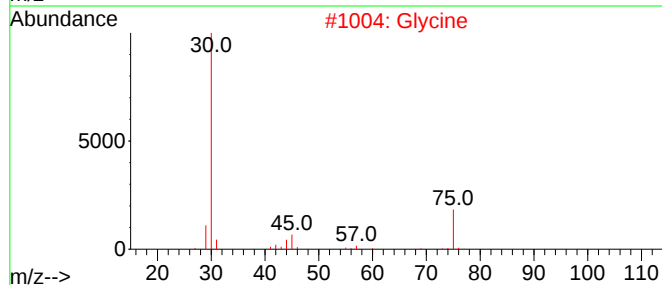
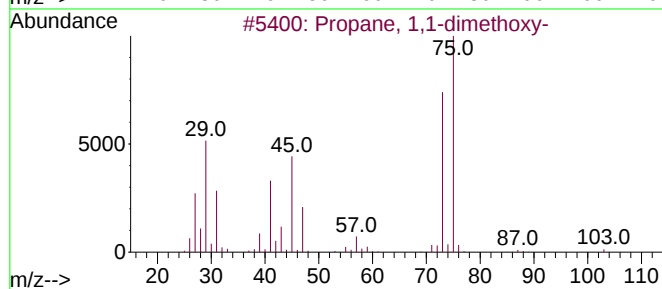
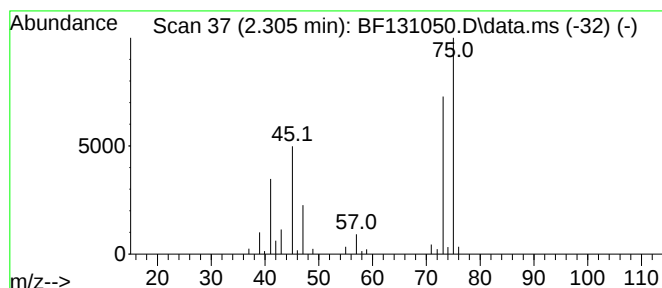
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.305 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.305	2.01 ng	53506	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	47
2			Glycine	75	C2H5NO2	000056-40-6	9
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	7
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



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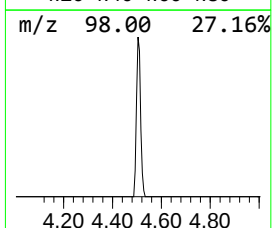
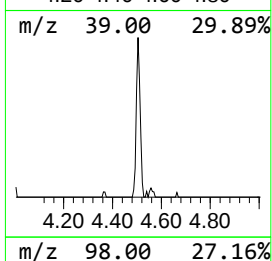
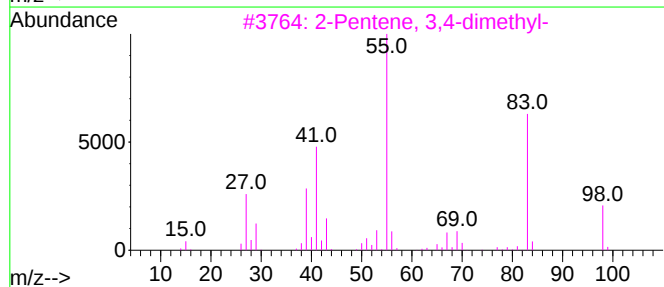
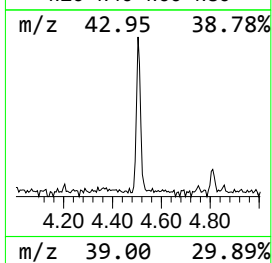
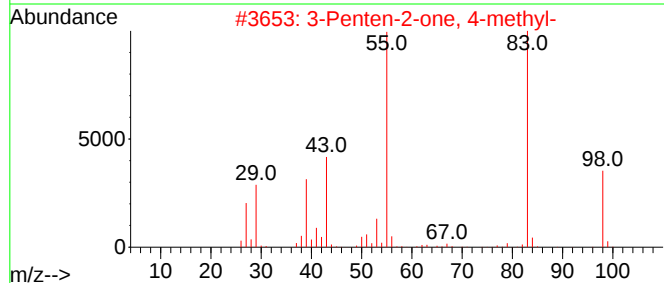
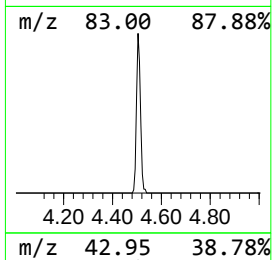
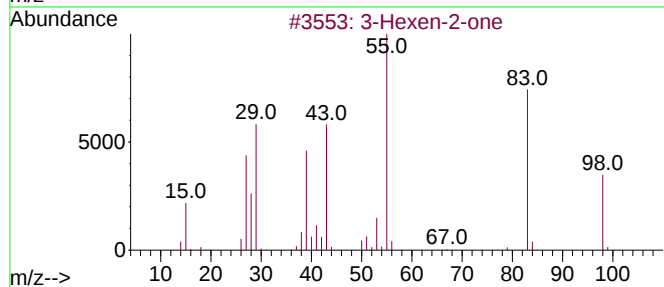
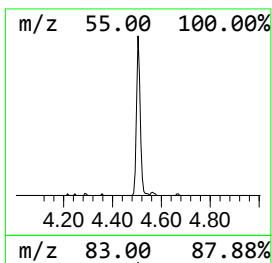
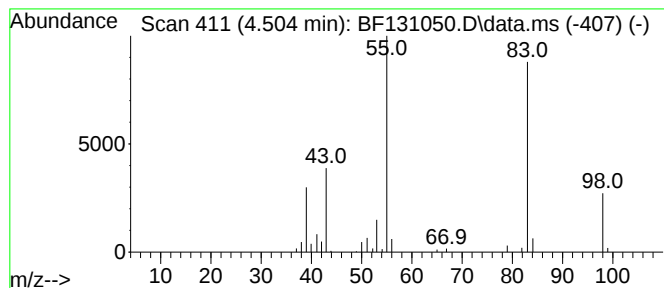
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Hexen-2-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	2.56 ng	68348	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
4			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	86
5			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86



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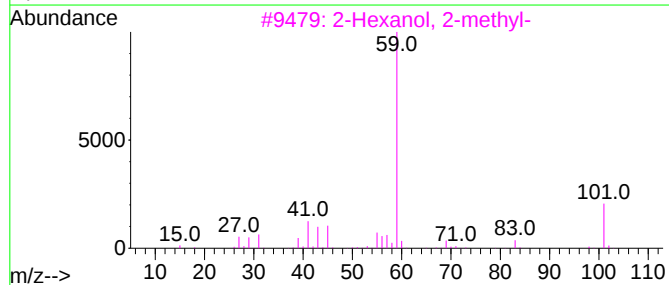
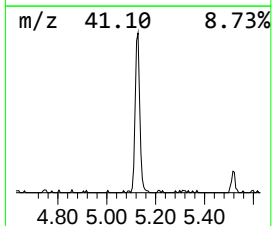
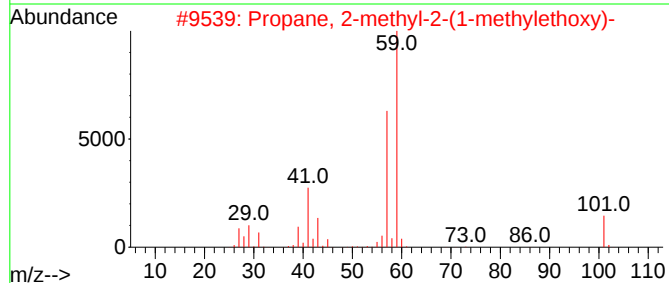
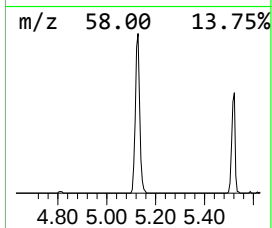
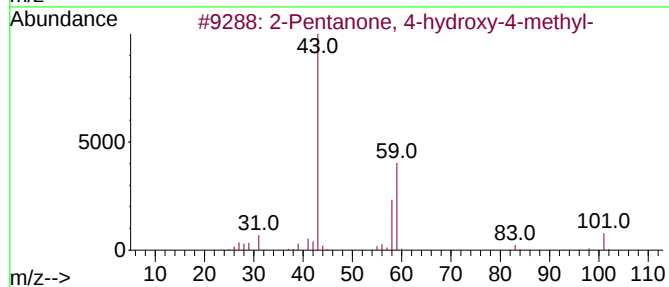
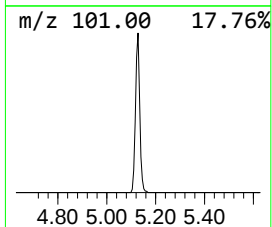
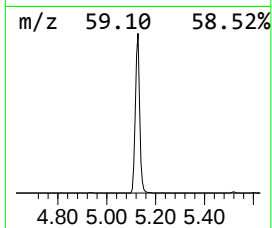
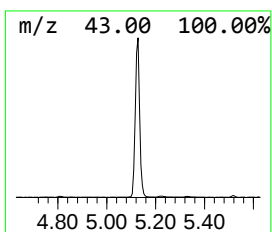
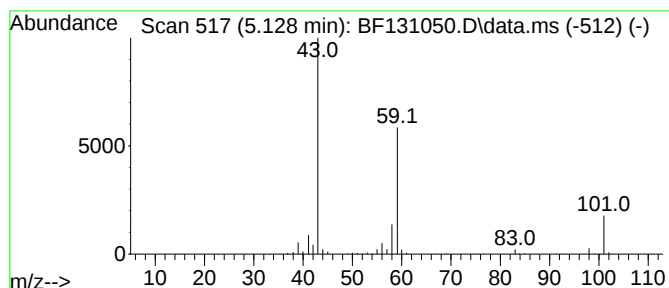
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	18.41 ng	490807	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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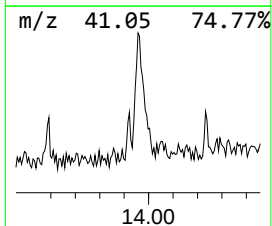
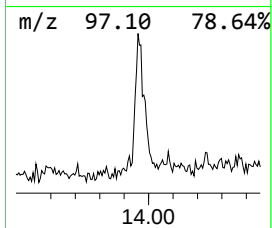
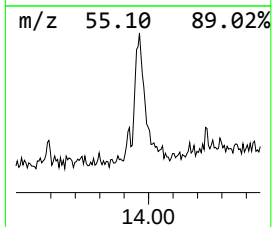
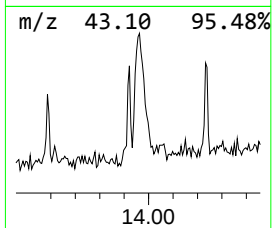
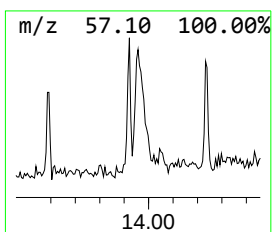
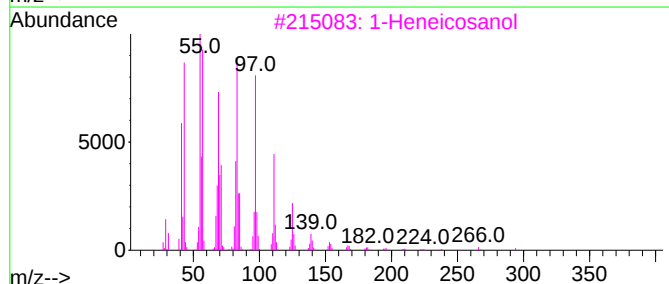
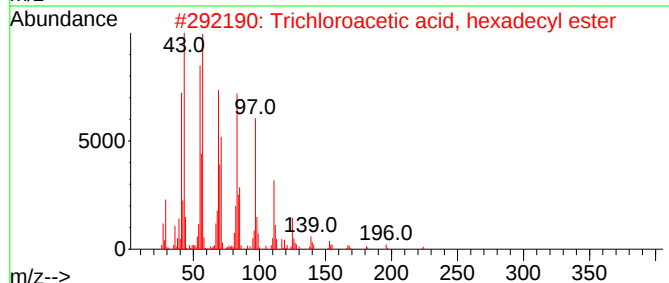
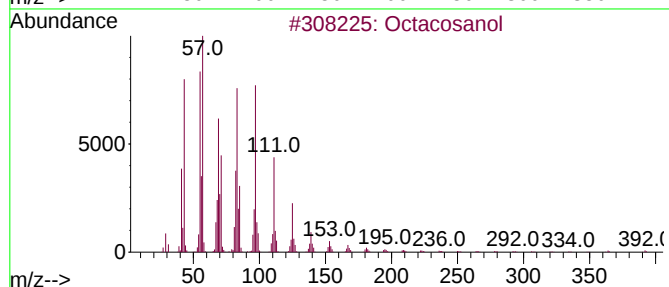
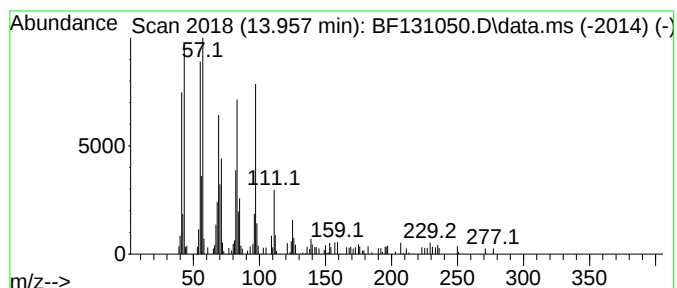
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	5.94 ng	167116	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



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Data File : BF131050.D
Acq On : 07 Nov 2022 18:54
Operator : CG\JU
Sample : N5415-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

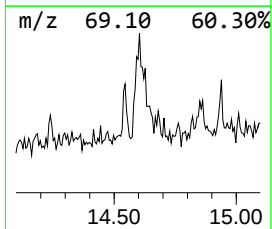
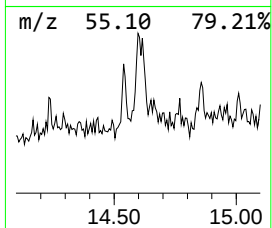
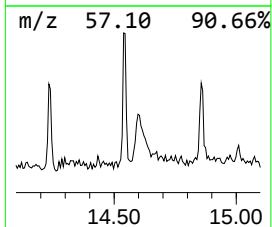
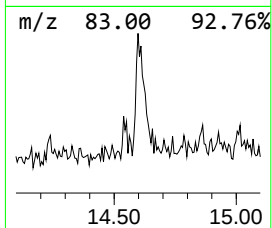
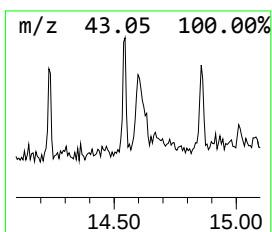
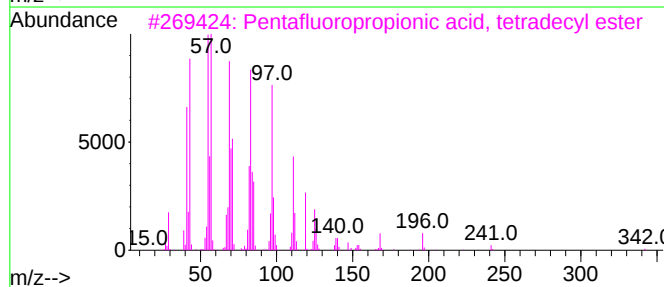
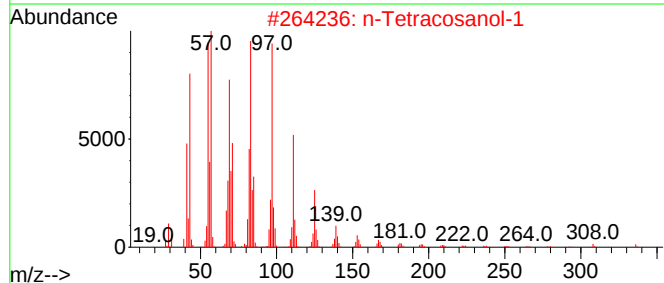
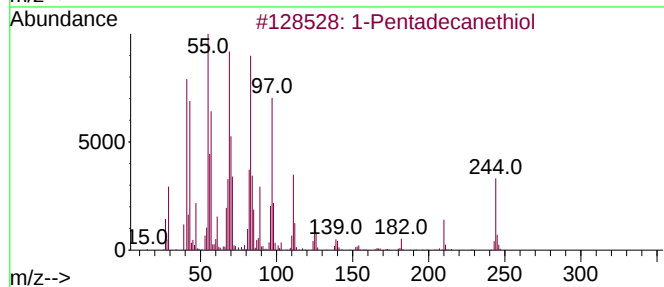
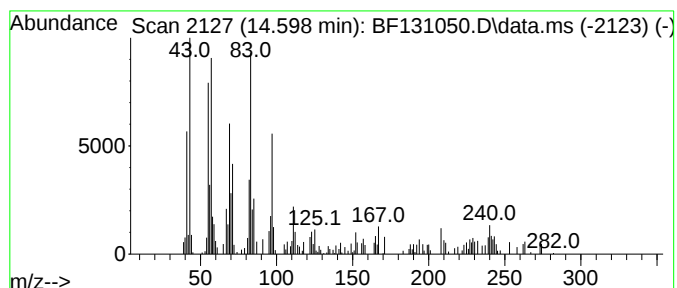
Instrument :
BNA_F
ClientSampleId :
R-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Pentadecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.598	3.65 ng	102762	Chrysene-d12		14.080	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol		244	C15H32S	025276-70-4	84
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	74
3	Pentafluoropropionic acid, tetra...		360	C17H29F5O2	006222-06-6	70
4	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	70
5	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131050.D
Acq On : 07 Nov 2022 18:54
Operator : CG\JU
Sample : N5415-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-16

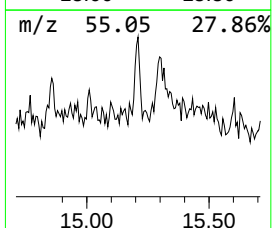
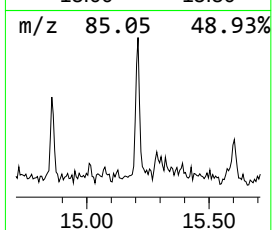
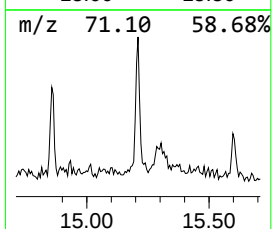
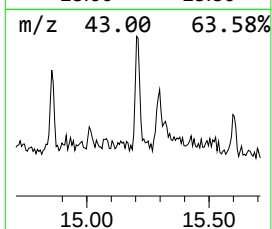
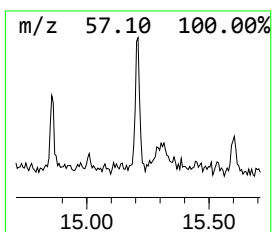
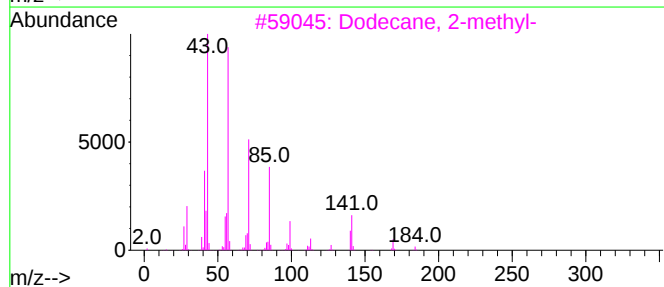
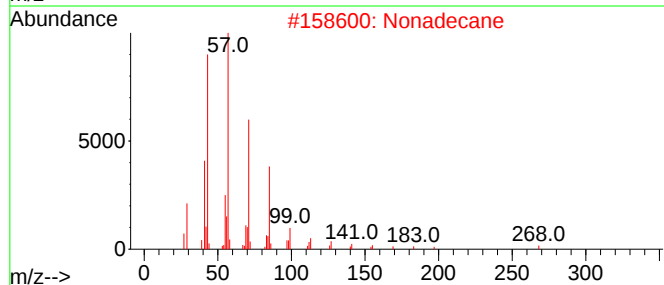
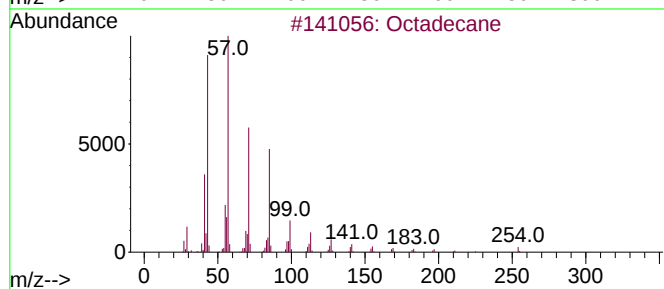
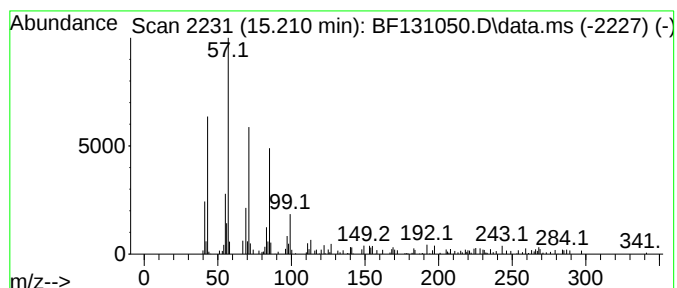
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	2.52 ng	57949	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	87
2			Nonadecane	268	C19H40	000629-92-5	83
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
4			2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5			Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131050.D
Acq On : 07 Nov 2022 18:54
Operator : CG\JU
Sample : N5415-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.193	29.3	ng	782003	1	6.898	533289	20.0
unknown2.305	2.305	2.0	ng	53506	1	6.898	533289	20.0
3-Hexen-2-one	4.504	2.6	ng	68348	1	6.898	533289	20.0
2-Pentanone, 4-...	5.128	18.4	ng	490807	1	6.898	533289	20.0
Octacosanol	13.957	5.9	ng	167116	5	14.080	562580	20.0
1-Pentadecanethiol	14.598	3.6	ng	102762	5	14.080	562580	20.0
Octadecane	15.210	2.5	ng	57949	6	15.580	460535	20.0