

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120222\
 Data File : BF131501.D
 Acq On : 02 Dec 2022 18:02
 Operator : CG\JU
 Sample : N5847-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-40-GW-01

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131501.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	19	28	34	rVB	1799480	2435475	85.39%	12.757%
2	5.152	515	521	528	rVB	374427	444066	15.57%	2.326%
3	5.546	582	588	591	rBV	1335716	1360840	47.71%	7.128%
4	5.940	651	655	661	rVB	49206	41540	1.46%	0.218%
5	6.546	753	758	761	rBV	1140728	1049380	36.79%	5.497%
6	6.928	819	823	826	rBV	491808	438349	15.37%	2.296%
7	7.493	913	919	922	rBV	1419572	1533286	53.76%	8.031%
8	8.216	1033	1042	1045	rBV	660439	588335	20.63%	3.082%
9	9.298	1220	1226	1229	rBV	3093437	2852209	100.00%	14.940%
10	9.981	1337	1342	1345	rBV	839266	678396	23.78%	3.553%
11	10.775	1470	1477	1480	rBV	1937996	1783942	62.55%	9.344%
12	11.422	1584	1587	1590	rVB	51934	41114	1.44%	0.215%
13	11.475	1592	1596	1599	rBV	750852	612614	21.48%	3.209%
14	11.763	1640	1645	1652	rBV7	13087	33445	1.17%	0.175%
15	11.998	1681	1685	1689	rBV	62201	56416	1.98%	0.296%
16	12.392	1748	1752	1754	rBV	84494	74948	2.63%	0.393%
17	12.557	1774	1780	1782	rBV	68120	72746	2.55%	0.381%
18	12.716	1804	1807	1811	rVB	168690	144640	5.07%	0.758%
19	12.875	1831	1834	1838	rBV	446421	380313	13.33%	1.992%
20	13.075	1863	1868	1874	rBV	2632362	2476880	86.84%	12.974%
21	13.939	2012	2015	2018	rBV3	37453	38287	1.34%	0.201%
22	14.016	2023	2028	2040	rBV4	58973	198165	6.95%	1.038%
23	14.127	2040	2047	2051	rBV	593955	582580	20.43%	3.051%
24	14.227	2059	2064	2069	rVB	103485	113573	3.98%	0.595%
25	14.598	2121	2127	2131	rBV	34778	39571	1.39%	0.207%
26	14.998	2191	2195	2200	rBV	200673	200977	7.05%	1.053%
27	15.274	2239	2242	2247	rBV2	31342	37973	1.33%	0.199%
28	15.657	2301	2307	2319	rVB	380969	560207	19.64%	2.934%
29	16.151	2382	2391	2396	rBV	36397	65869	2.31%	0.345%
30	16.692	2475	2483	2491	rBV3	33454	77539	2.72%	0.406%
31	17.333	2587	2592	2598	rVB2	19935	37063	1.30%	0.194%
32	18.080	2713	2719	2730	rVB4	15124	40939	1.44%	0.214%

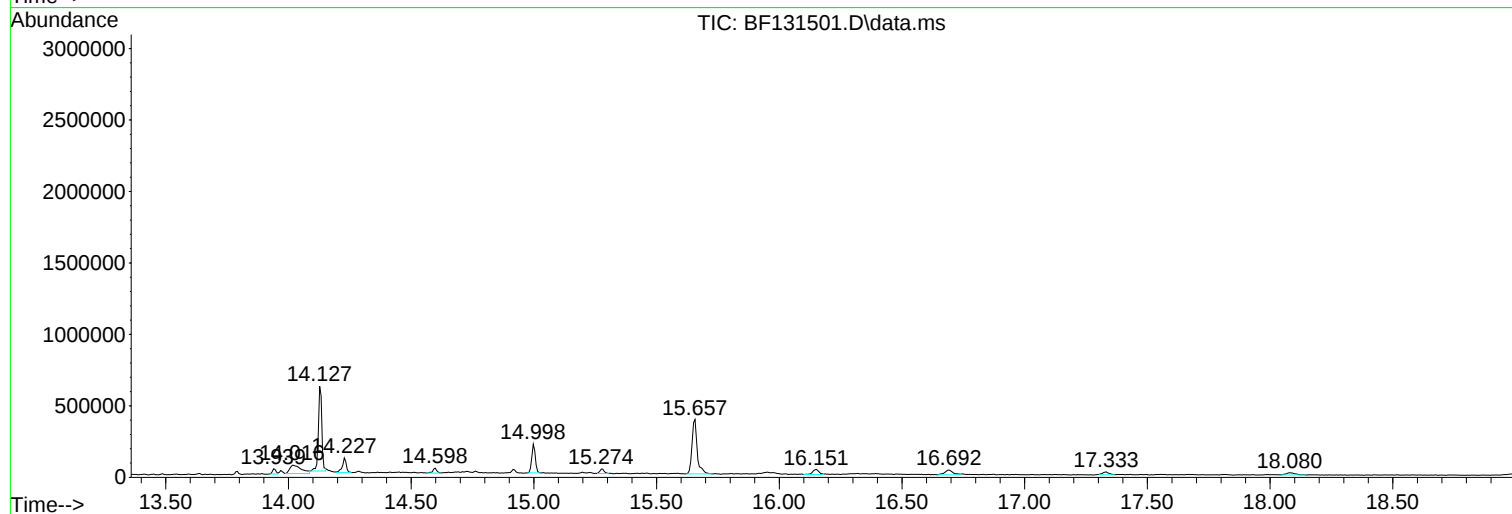
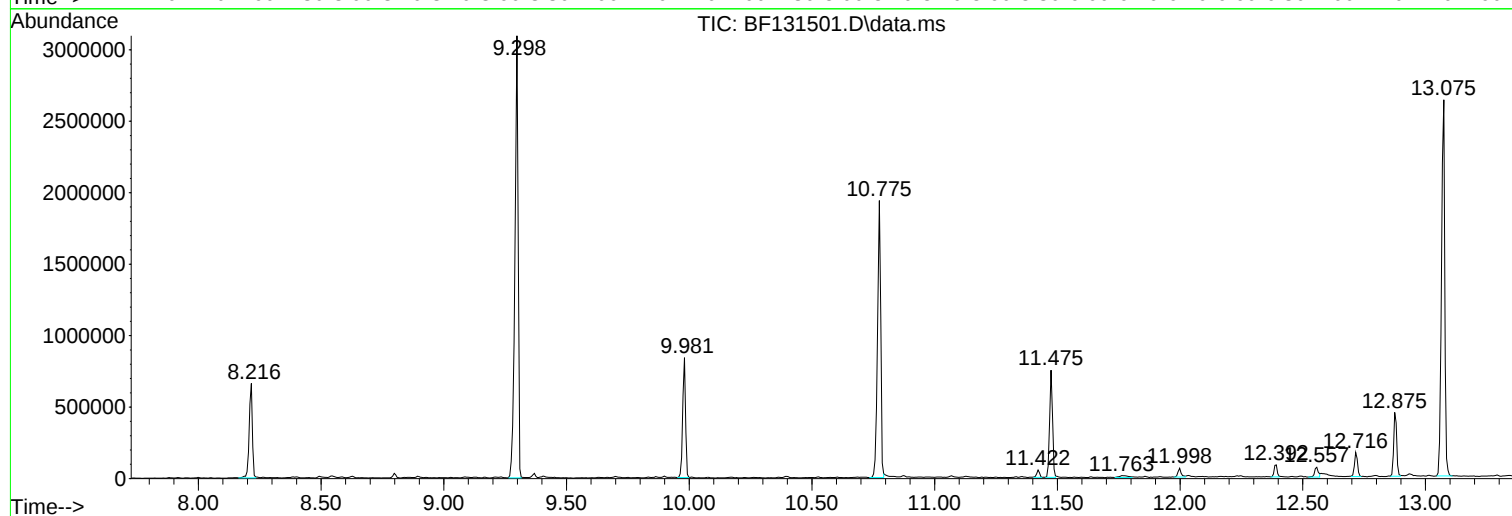
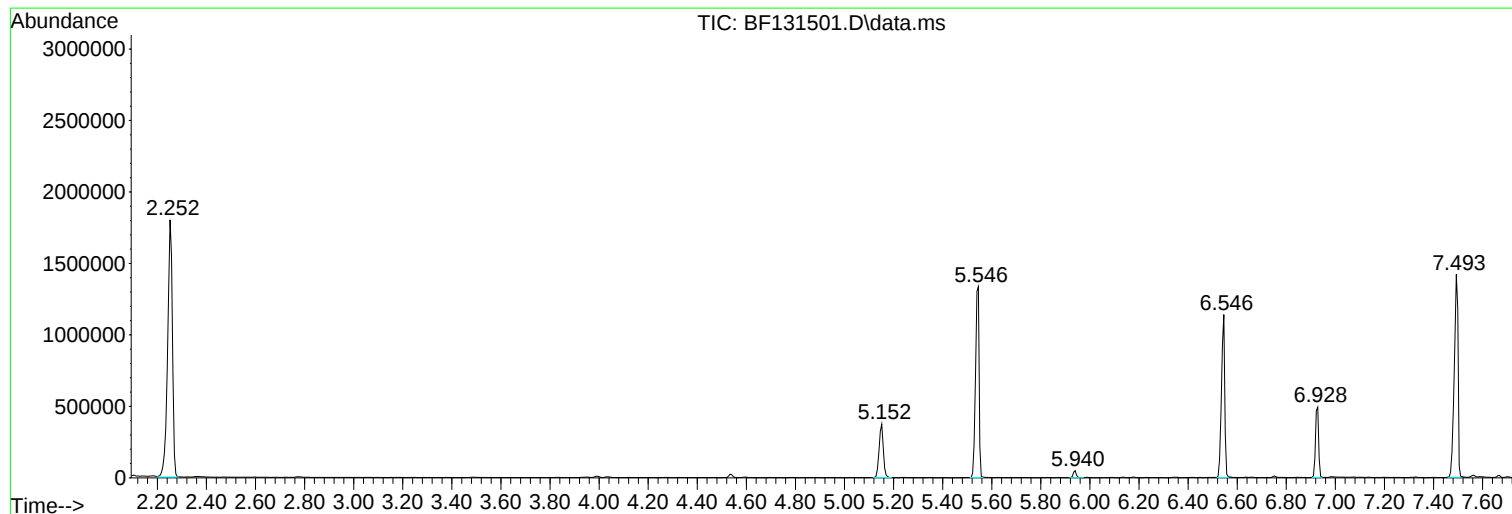
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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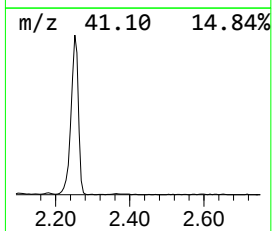
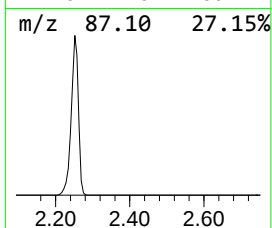
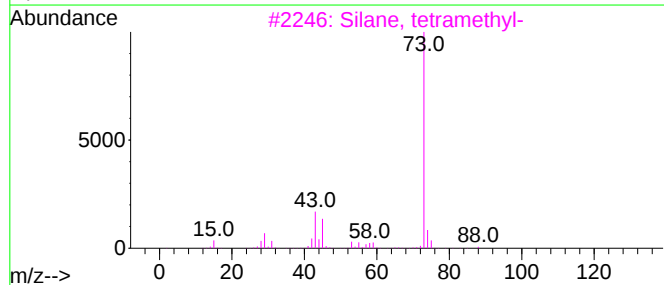
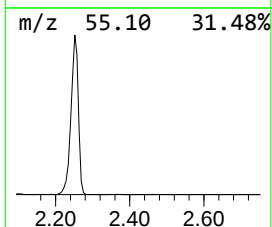
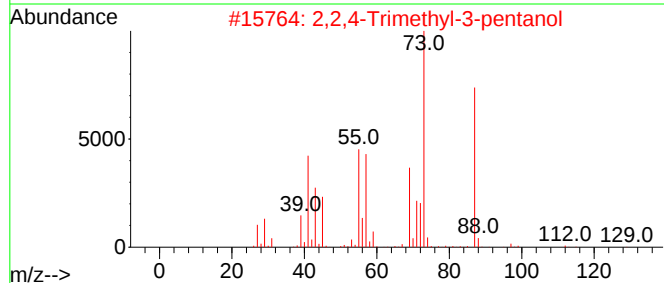
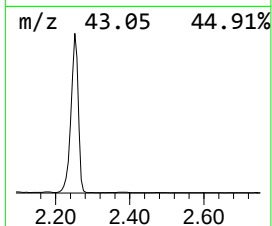
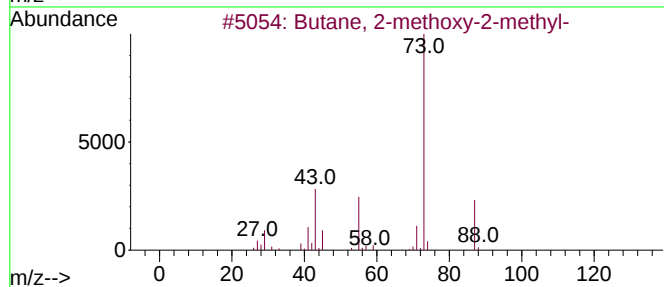
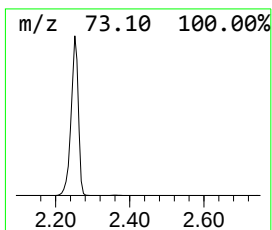
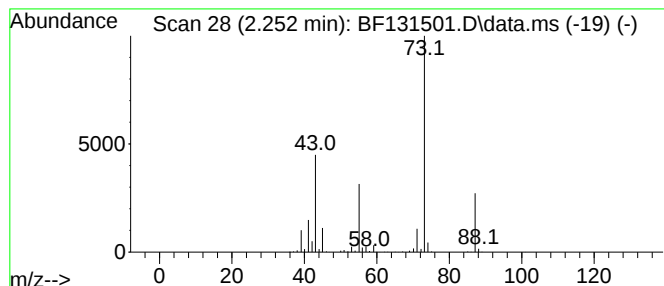
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.252	111.12 ng	2435480	1,4-Dichlorobenzene-d4	6.928

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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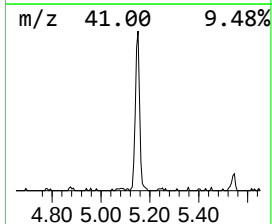
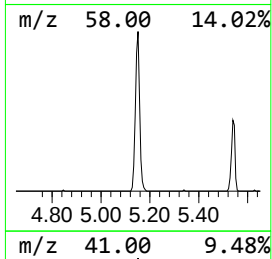
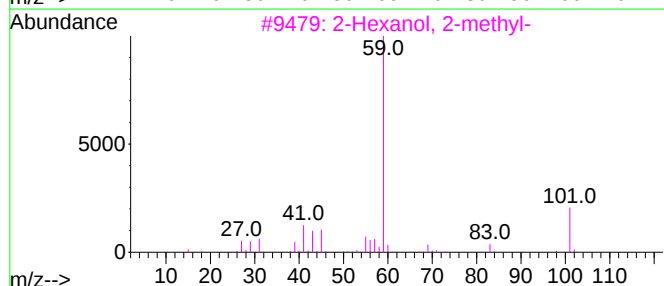
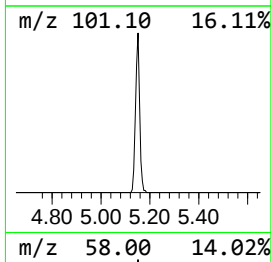
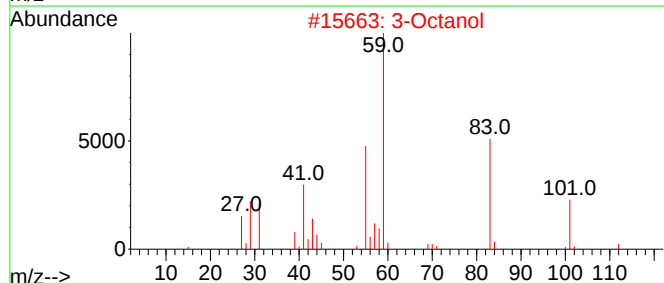
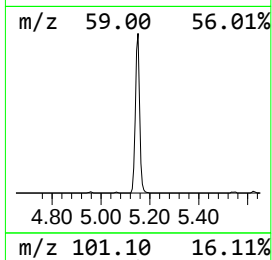
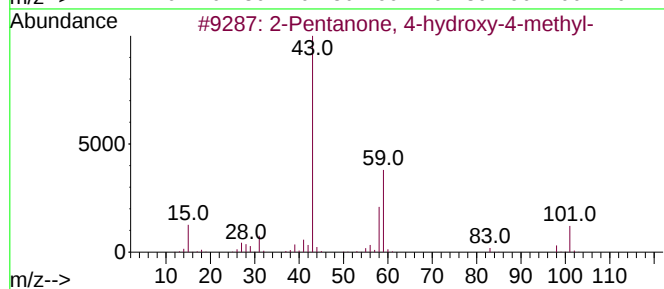
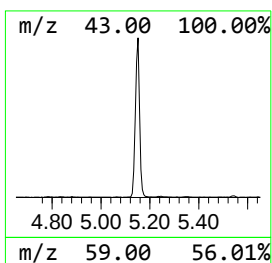
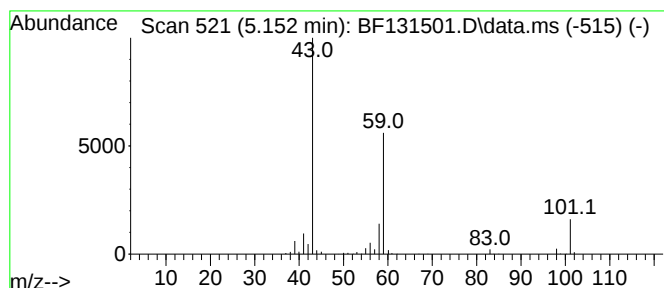
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.152	20.26 ng	444066	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Octanol	130	C8H18O	000589-98-0	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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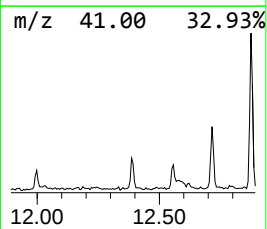
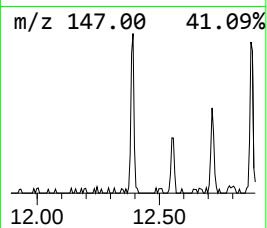
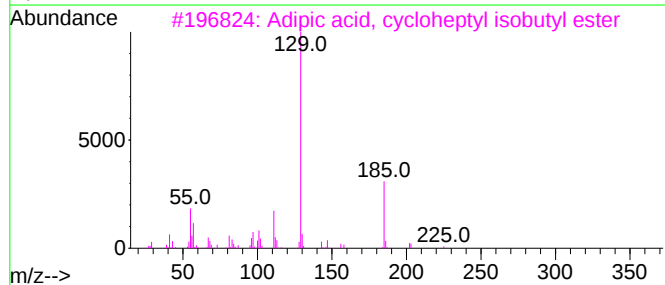
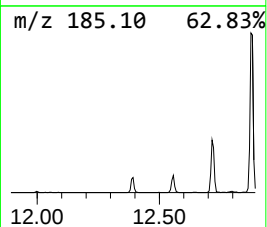
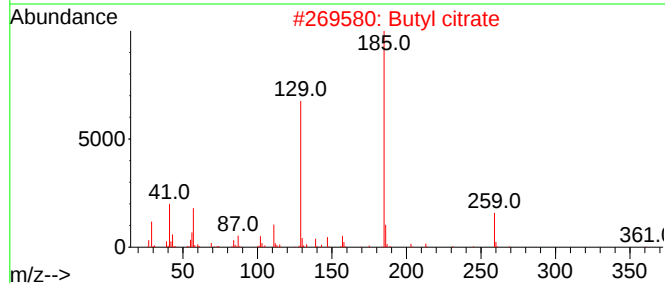
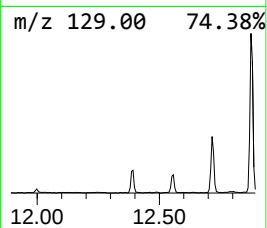
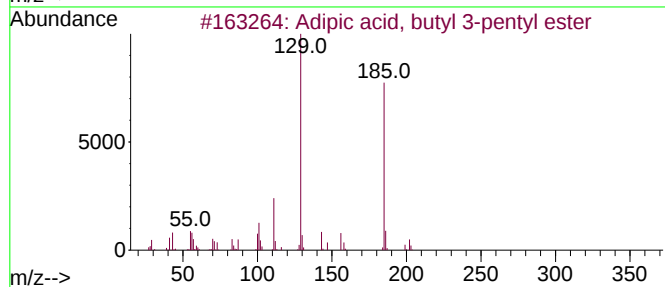
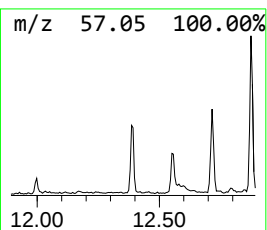
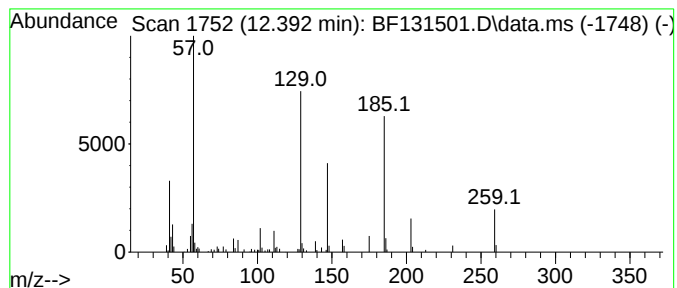
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.392 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	2.45 ng	74948	Phenanthrene-d10	11.475

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	47
2		Butyl citrate	360	C18H32O7	000077-94-1	43
3		Adipic acid, cycloheptyl isobuty...	298	C17H30O4	1000324-71-5	40
4		Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	40
5		Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	38



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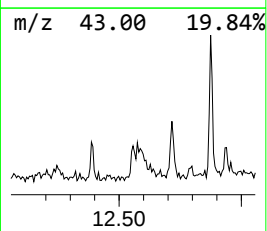
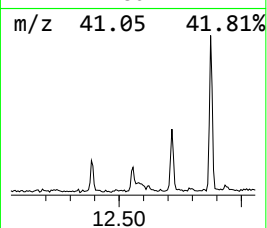
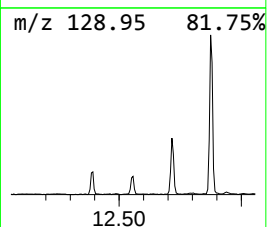
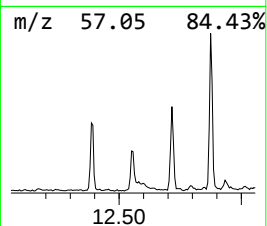
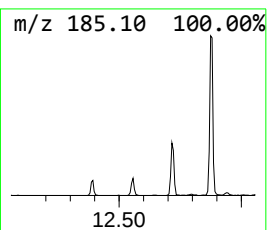
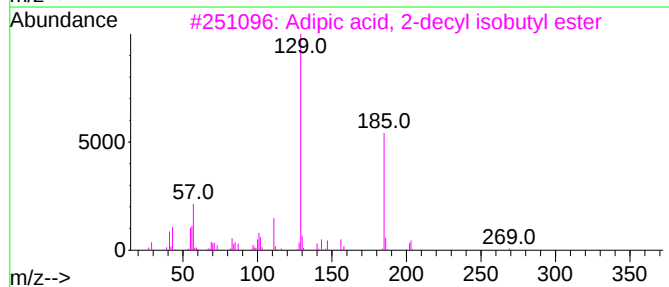
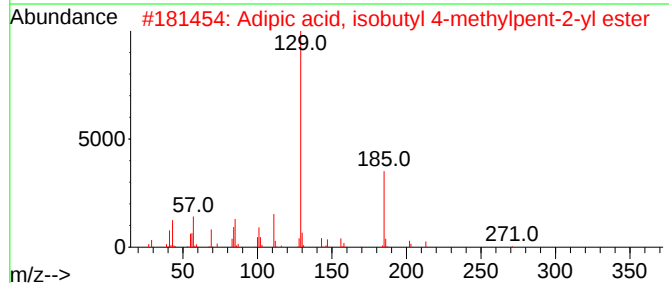
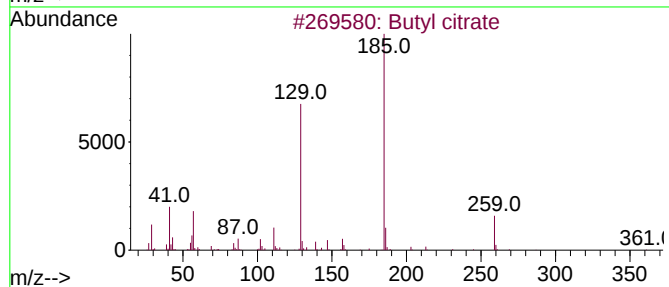
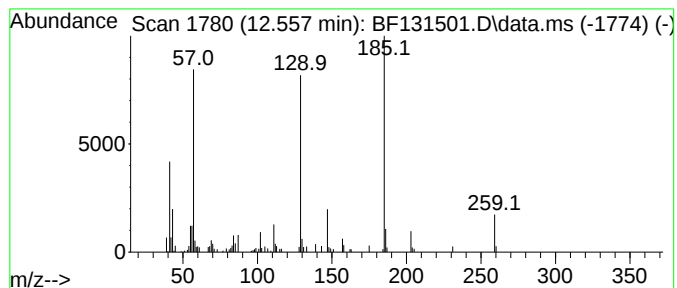
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butyl citrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	2.37 ng	72746	Phenanthrene-d10	11.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	83
2			Adipic acid, isobutyl 4-methylpe...	286	C16H30O4	1000353-50-1	72
3			Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	64
4			Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	59
5			Adipic acid, butyl 2,4-dimethylp...	300	C17H32O4	1000349-77-7	53



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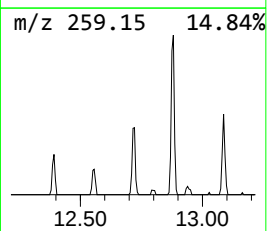
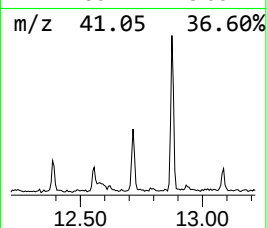
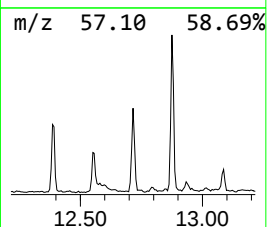
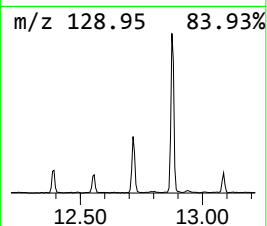
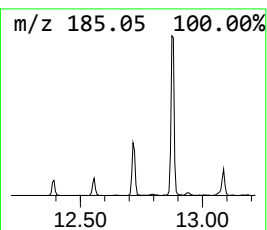
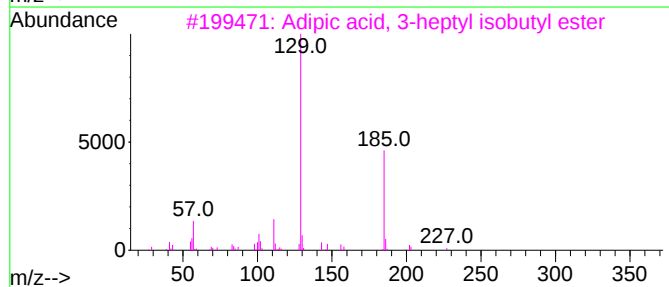
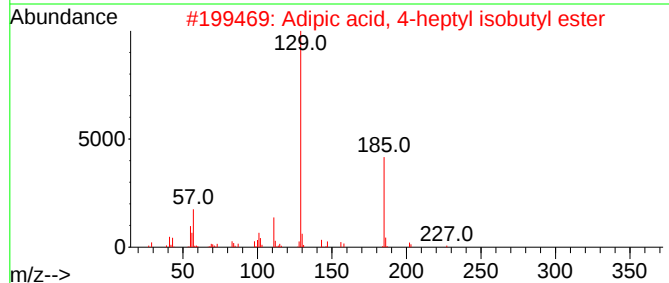
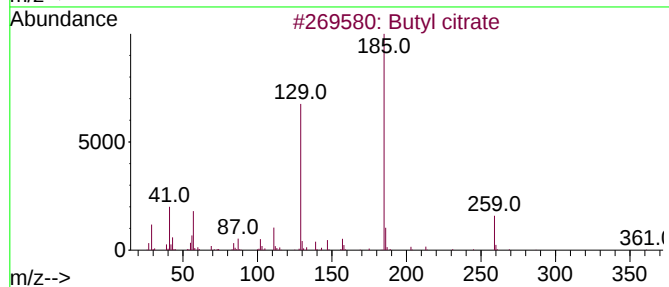
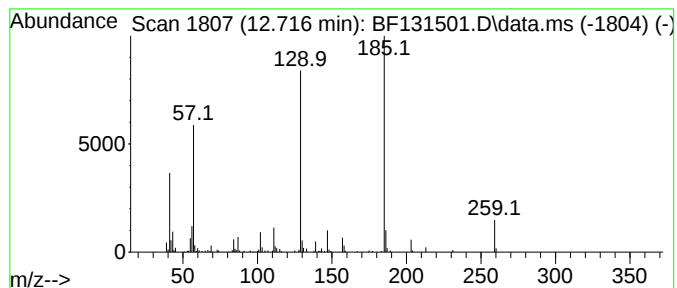
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Peak Number 5 Adipic acid, 4-heptyl isobu... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.716	4.72 ng	144640	Phenanthrene-d10	11.475	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	72
3	Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	72
4	Adipic acid, butyl isobutyl ester	258	C14H26O4	1010324-09-3	59
5	Dibutyl adipate	258	C14H26O4	000105-99-7	50



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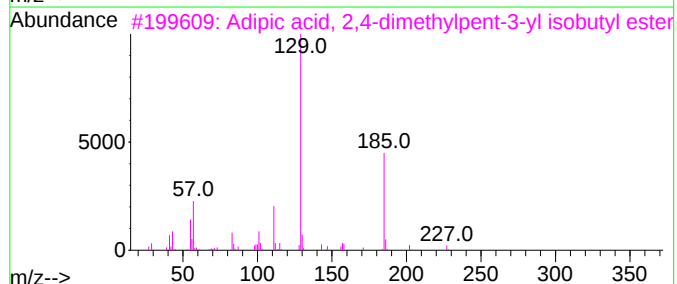
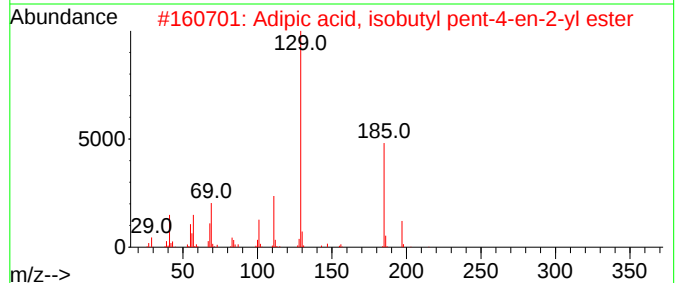
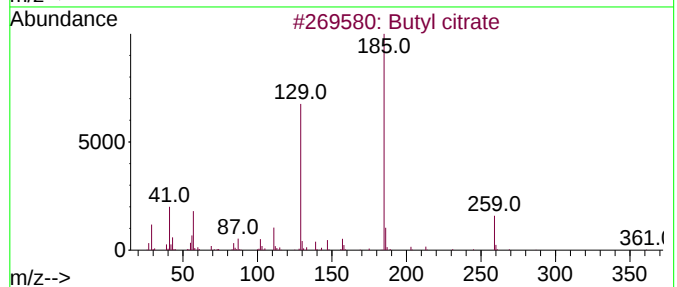
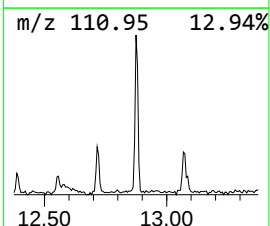
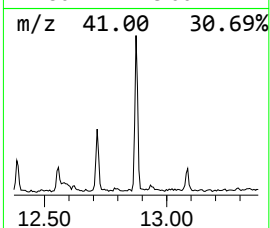
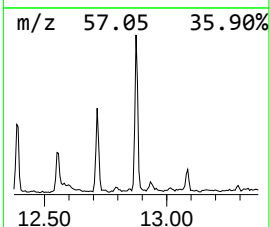
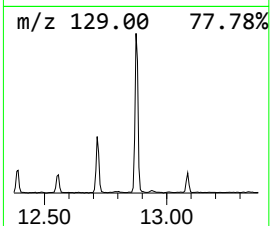
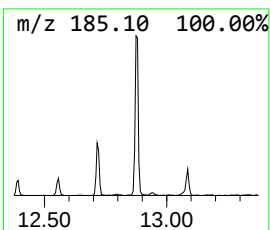
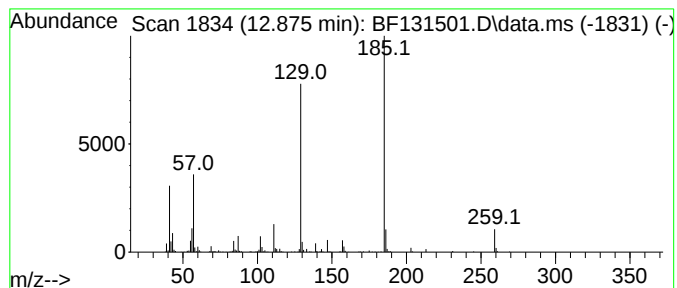
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Adipic acid, isobutyl pent-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.874	13.06 ng	380313	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, isobutyl pent-4-en-...	270	C15H26O4	1000354-11-8	72
3			Adipic acid, 2,4-dimethylpent-3-...	300	C17H32O4	1000349-77-6	43
4			Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	40
5			Adipic acid, butyl 2-hexyl ester	286	C16H30O4	1000353-71-0	38



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Data File : BF131501.D
Acq On : 02 Dec 2022 18:02
Operator : CG\JU
Sample : N5847-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

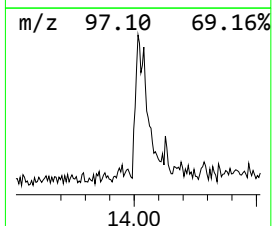
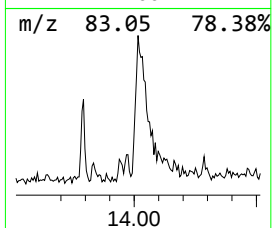
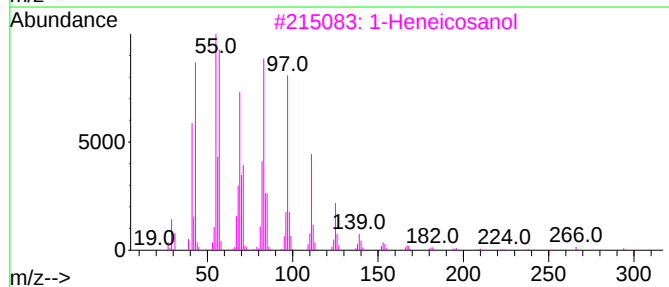
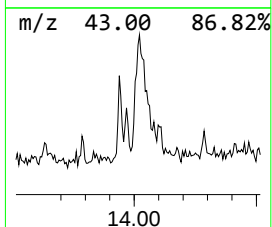
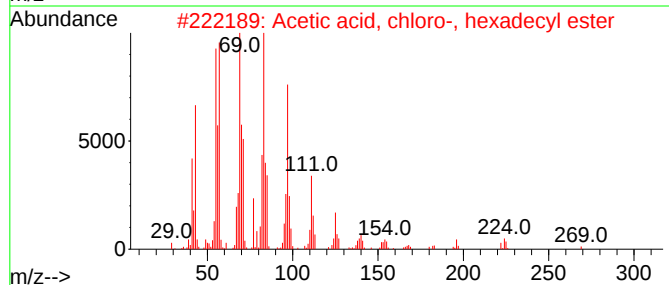
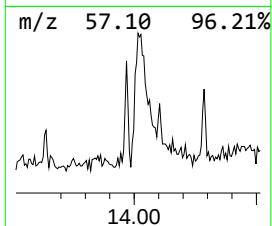
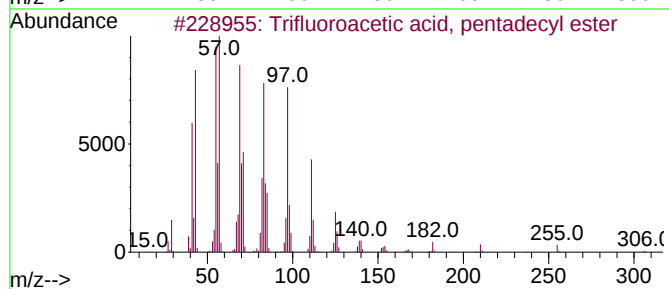
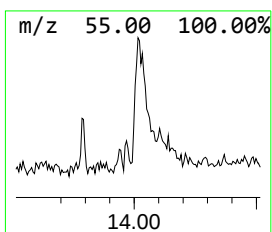
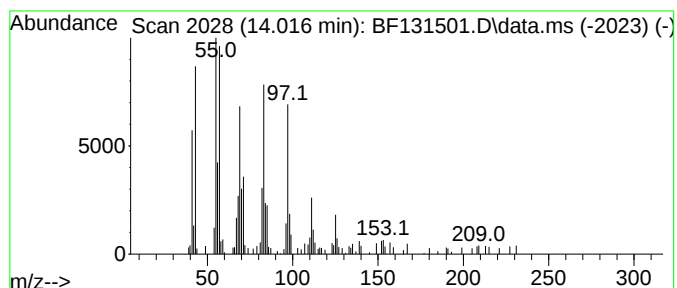
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.016	6.80 ng	198165	Chrysene-d12	14.127	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120222\
Data File : BF131501.D
Acq On : 02 Dec 2022 18:02
Operator : CG\JU
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Instrument :
BNA_F
ClientSampleId :
B-40-GW-01

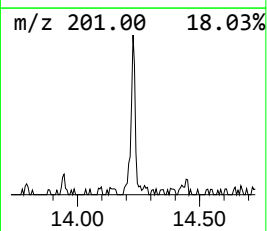
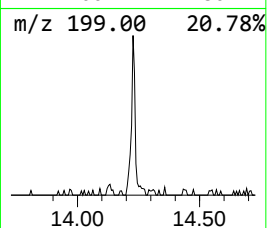
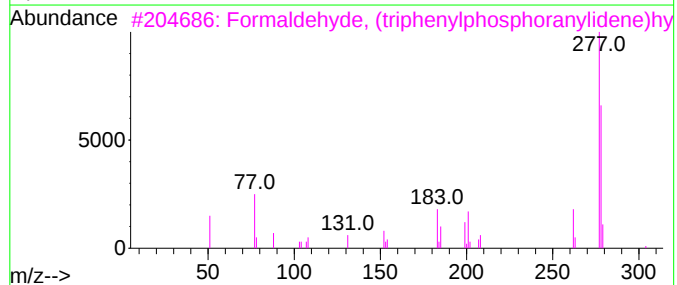
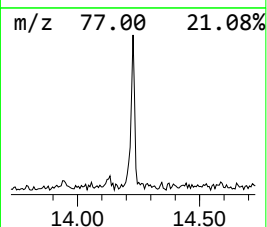
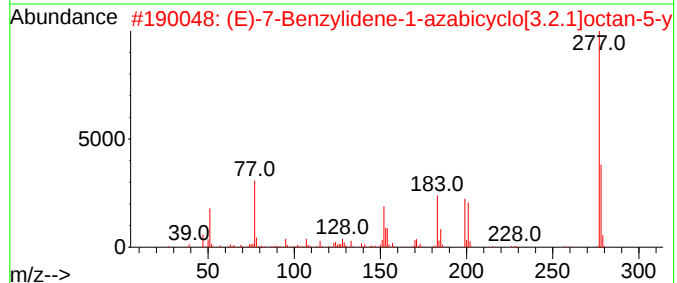
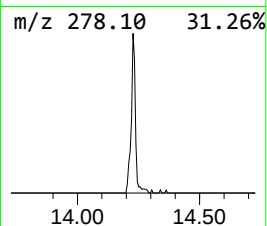
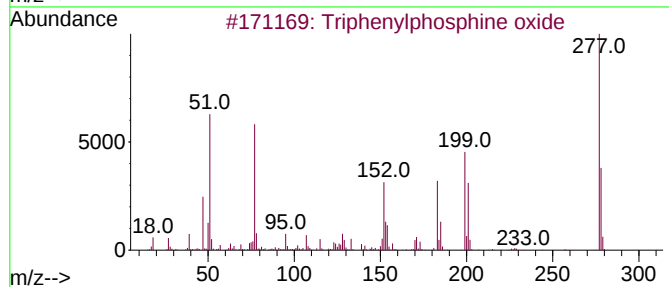
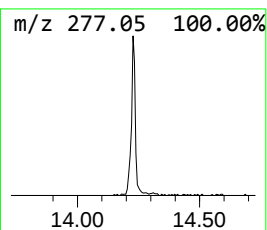
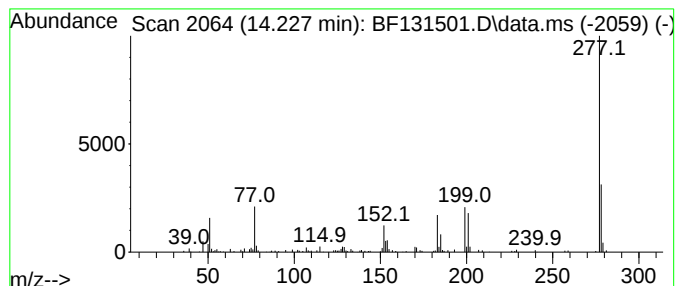
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	3.90 ng	113573	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
5			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120222\
Data File : BF131501.D
Acq On : 02 Dec 2022 18:02
Operator : CG\JU
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ALS Vial : 10 Sample Multiplier: 1

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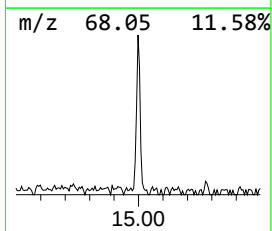
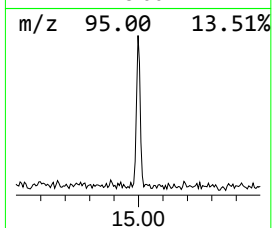
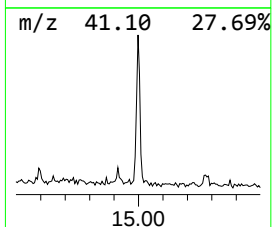
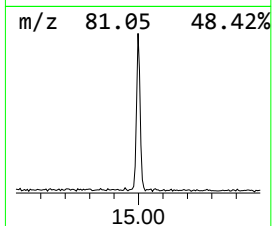
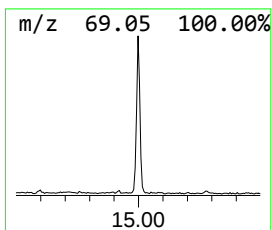
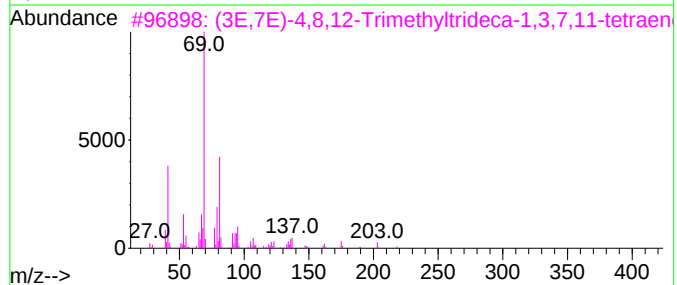
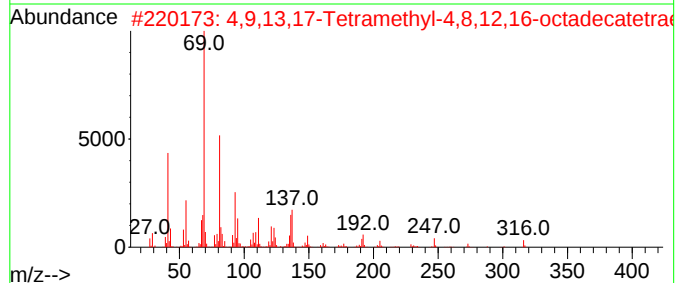
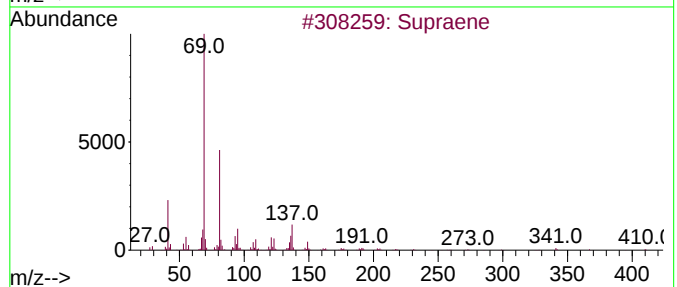
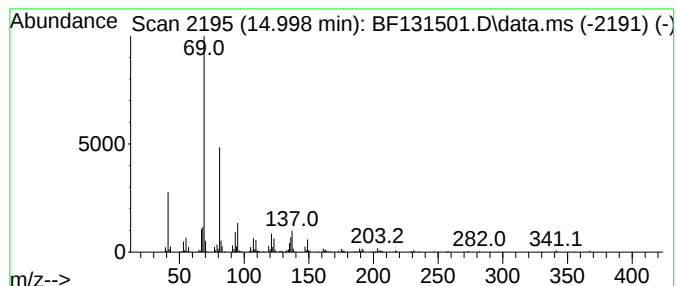
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	7.18 ng	200977	Perylene-d12	15.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3			(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	72
4			trans-Farnesol	222	C15H26O	000106-28-5	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120222\
Data File : BF131501.D
Acq On : 02 Dec 2022 18:02
Operator : CG\JU
Sample : N5847-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-40-GW-01

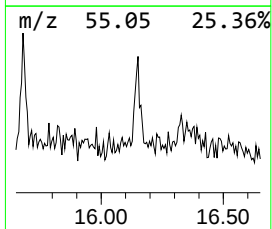
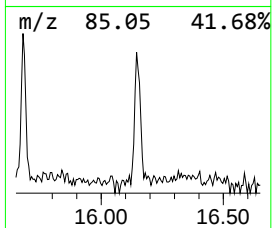
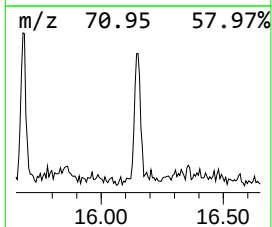
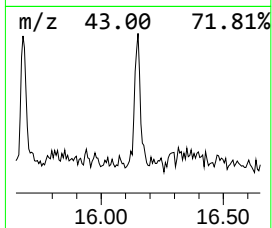
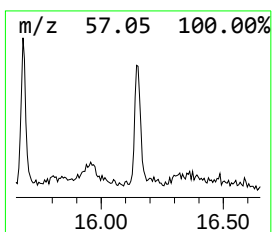
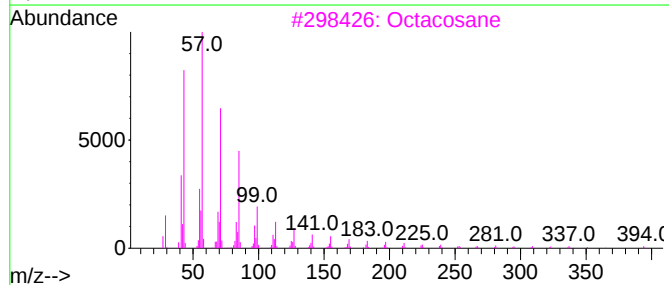
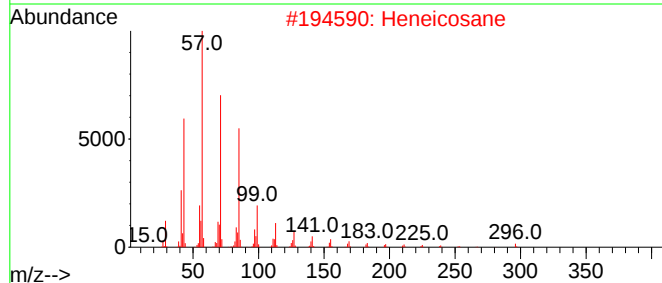
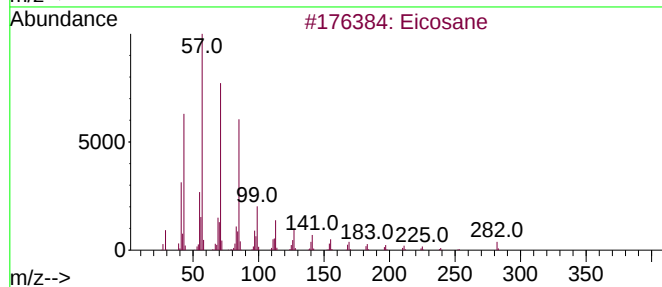
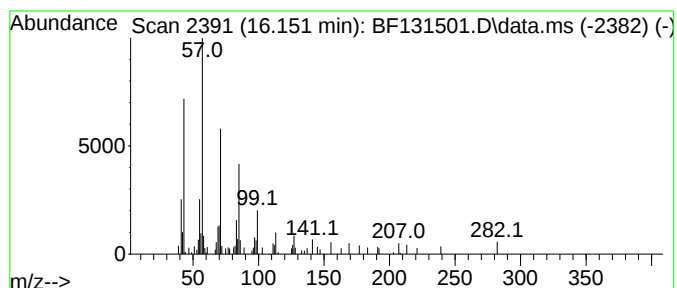
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.151	2.35 ng	65869	Perylene-d12	15.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Heneicosane	296	C21H44	000629-94-7	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Pentacosane	352	C25H52	000629-99-2	87
5			Triacontane	422	C30H62	000638-68-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120222\
Data File : BF131501.D
Acq On : 02 Dec 2022 18:02
Operator : CG\JU
Sample : N5847-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-40-GW-01

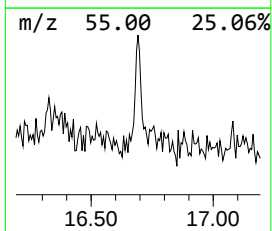
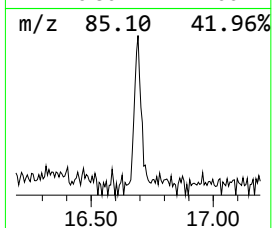
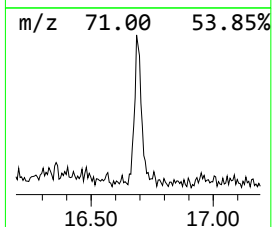
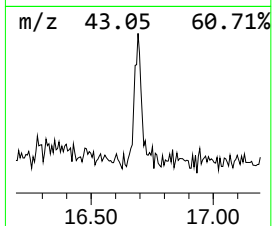
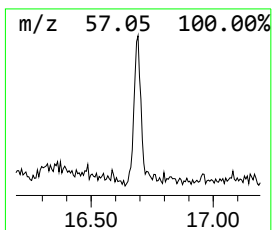
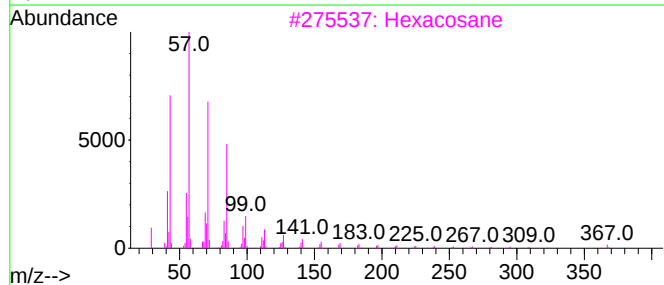
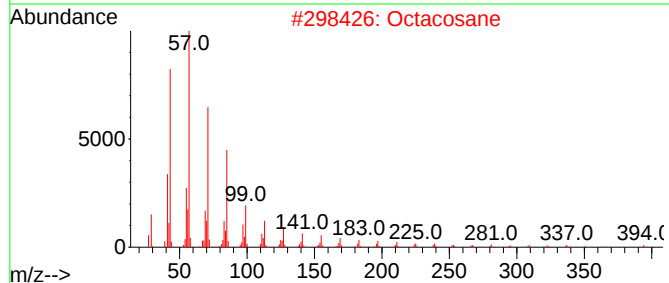
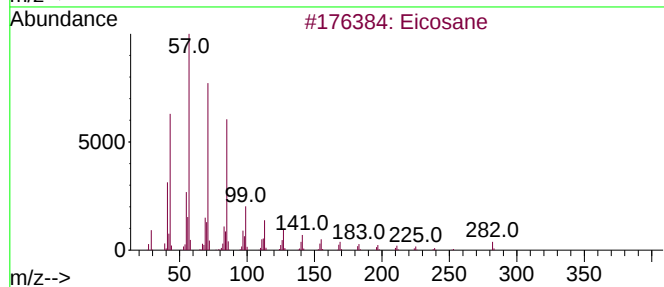
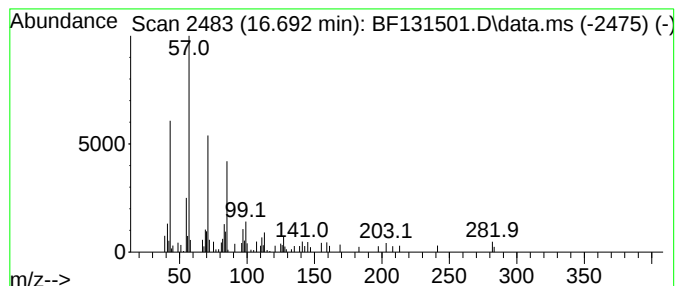
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.692	2.77 ng	77539	Perylene-d12	15.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Octacosane	394	C28H58	000630-02-4	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Hentriacontane	437	C31H64	000630-04-6	87
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120222\
Data File : BF131501.D
Acq On : 02 Dec 2022 18:02
Operator : CG\JU
Sample : N5847-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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

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

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					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.152	20.3	ng	444066	1	6.928	438349	20.0
unknown12.392	12.392	2.5	ng	74948	4	11.475	612614	20.0
Butyl citrate	12.557	2.4	ng	72746	4	11.475	612614	20.0
Adipic acid, 4-...	12.716	4.7	ng	144640	4	11.475	612614	20.0
Adipic acid, is...	12.874	13.1	ng	380313	5	14.127	582580	20.0
Trifluoroacetic...	14.016	6.8	ng	198165	5	14.127	582580	20.0
Triphenylphosph...	14.227	3.9	ng	113573	5	14.127	582580	20.0
Supraene	14.998	7.2	ng	200977	6	15.657	560207	20.0
Eicosane	16.151	2.4	ng	65869	6	15.657	560207	20.0
Octacosane	16.692	2.8	ng	77539	6	15.657	560207	20.0