

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020625\
 Data File : BF141486.D
 Acq On : 06 Feb 2025 18:00
 Operator : RC/JU
 Sample : Q1309-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2

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-BF020625.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141486.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	493	497	508	rVB	24469	41534	1.05%	0.157%
2	5.416	559	565	585	rBV	2125044	2955017	74.49%	11.157%
3	6.428	728	737	755	rBV	2202012	3126903	78.82%	11.806%
4	6.786	793	798	805	rBV	478602	583550	14.71%	2.203%
5	7.351	887	894	899	rBV	1466112	2035178	51.30%	7.684%
6	7.604	930	937	949	rBV	64929	90444	2.28%	0.341%
7	8.069	1010	1016	1021	rBV	607271	778174	19.62%	2.938%
8	9.145	1193	1199	1204	rBV	2756252	3609312	90.98%	13.627%
9	9.822	1308	1314	1327	rVB	722599	917089	23.12%	3.463%
10	10.539	1430	1436	1443	rBV	246498	311496	7.85%	1.176%
11	10.616	1443	1449	1464	rBV	1862775	2499909	63.02%	9.439%
12	10.980	1506	1511	1521	rBV	46505	70967	1.79%	0.268%
13	11.310	1562	1567	1572	rBV	761207	963073	24.28%	3.636%
14	11.421	1582	1586	1593	rBV	31395	48021	1.21%	0.181%
15	11.769	1640	1645	1652	rBV	73656	122609	3.09%	0.463%
16	11.851	1652	1659	1679	rVB	718244	1117768	28.18%	4.220%
17	12.551	1768	1778	1786	rBV	47246	105183	2.65%	0.397%
18	12.627	1787	1791	1804	rVV	122158	204660	5.16%	0.773%
19	12.904	1831	1838	1843	rBV	2940930	3967070	100.00%	14.978%
20	13.380	1911	1919	1927	rBV	119502	181210	4.57%	0.684%
21	13.810	1986	1992	2011	rBV4	110447	459022	11.57%	1.733%
22	13.951	2011	2016	2029	rVB	552518	760421	19.17%	2.871%
23	14.433	2094	2098	2102	rBV	40432	52681	1.33%	0.199%
24	14.815	2157	2163	2171	rVB	637822	859330	21.66%	3.244%
25	15.074	2202	2207	2212	rVB	28446	39881	1.01%	0.151%
26	15.415	2258	2265	2276	rBV	358554	585399	14.76%	2.210%

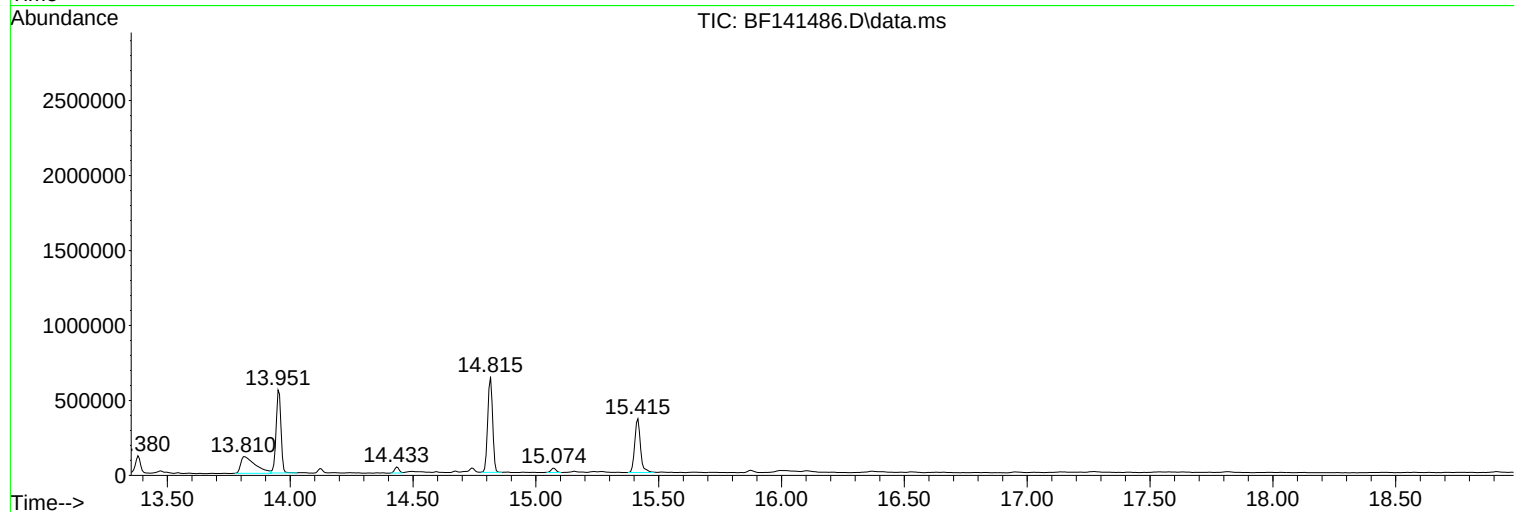
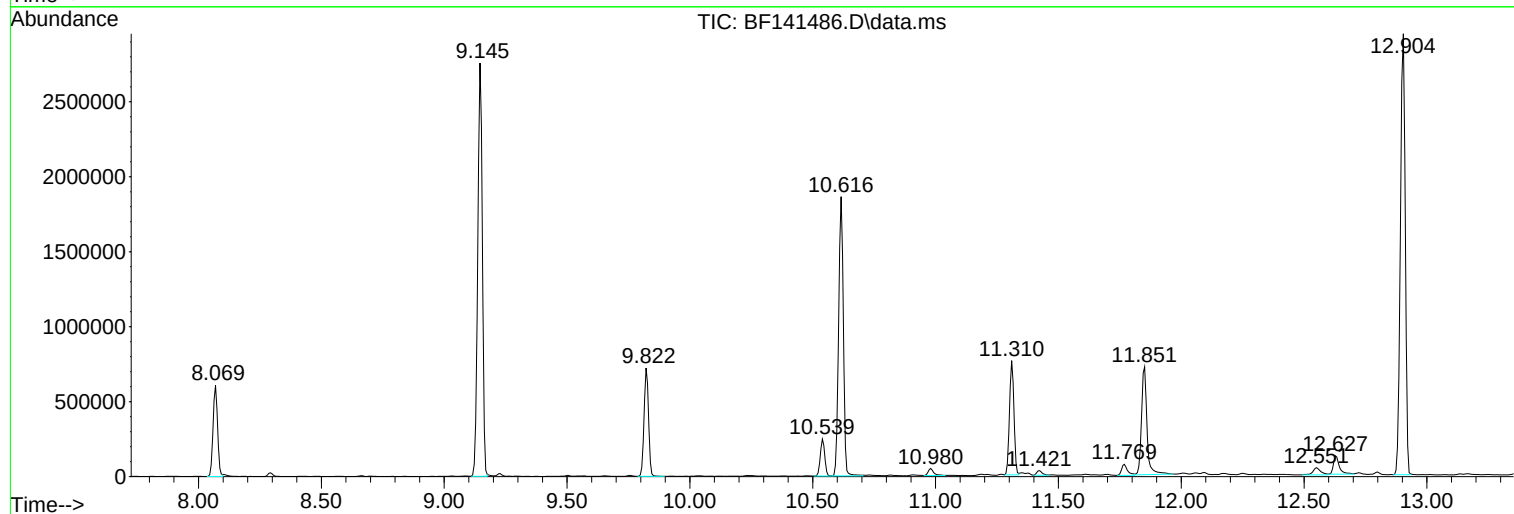
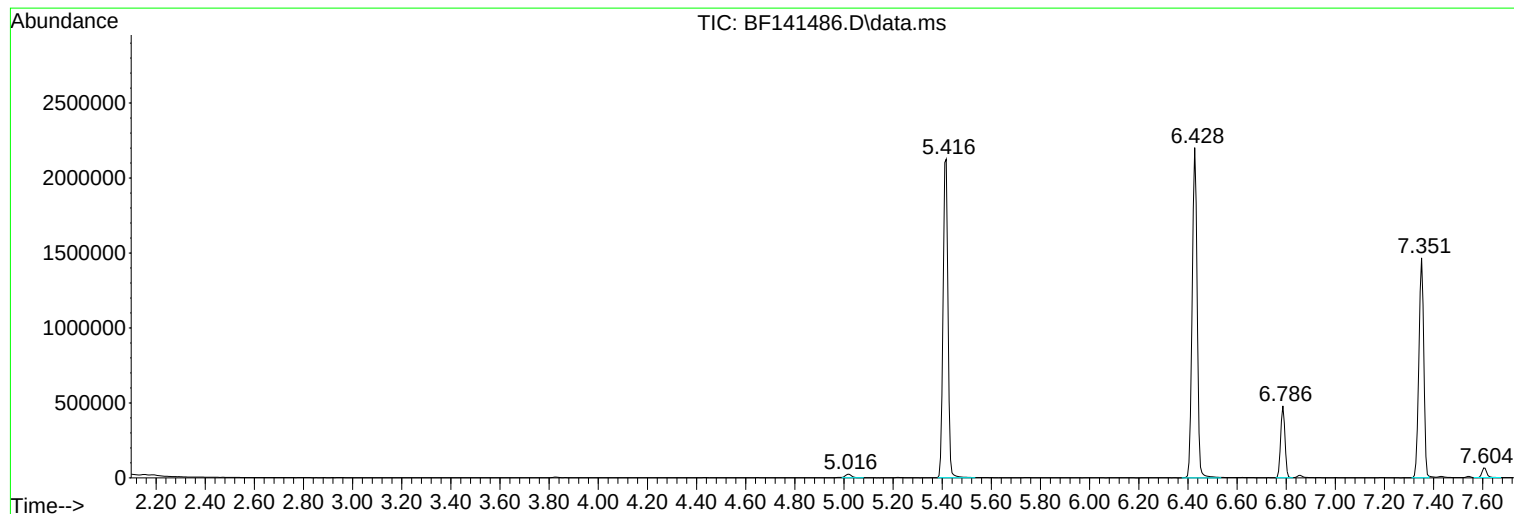
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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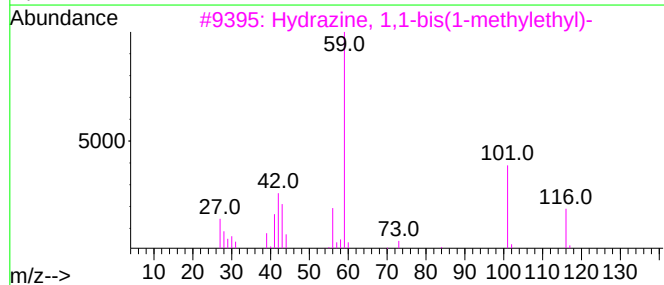
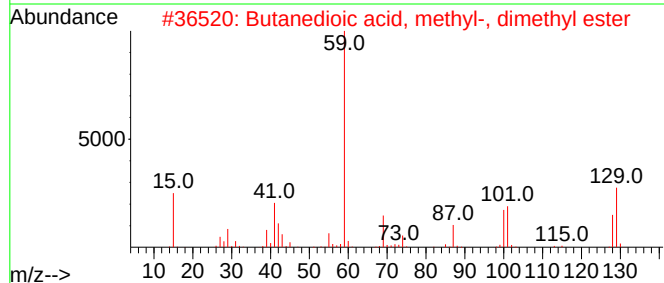
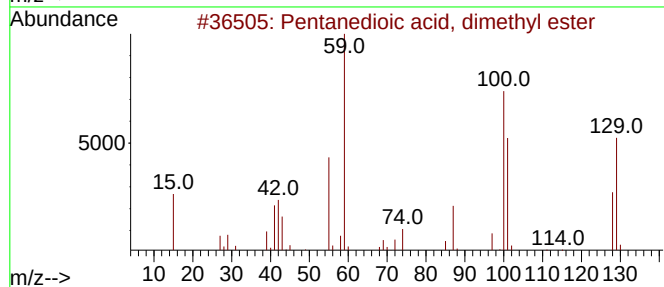
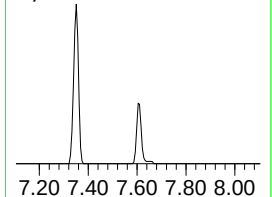
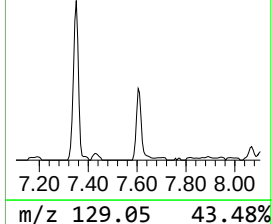
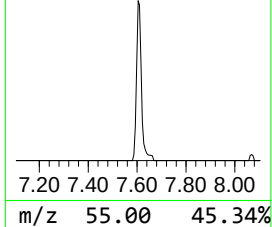
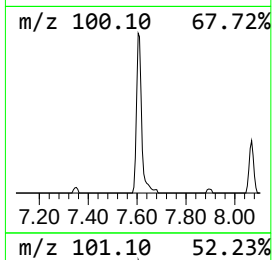
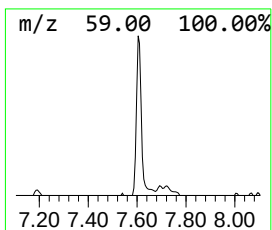
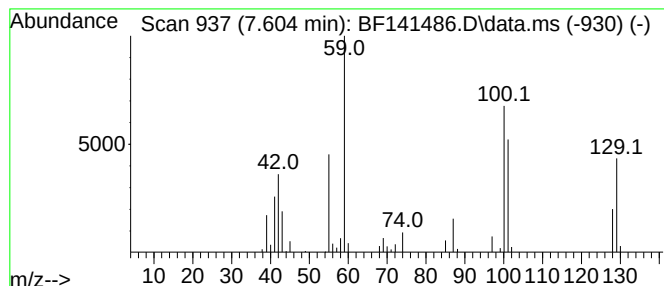
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Pentanedioic acid, dimethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.604	2.32 ng	90444	Naphthalene-d8	8.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	90
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	59
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	32
4			6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	14
5			Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	14



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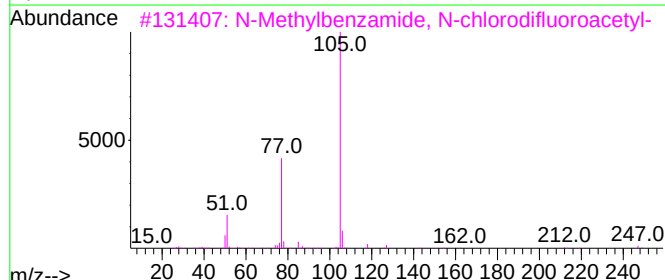
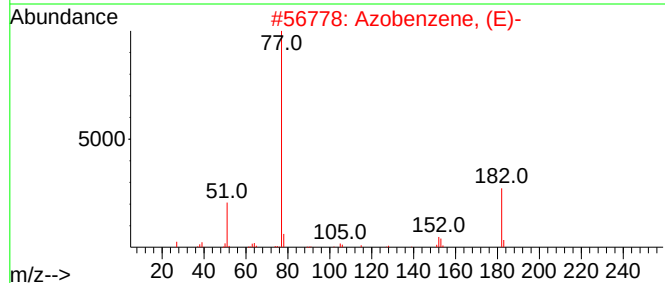
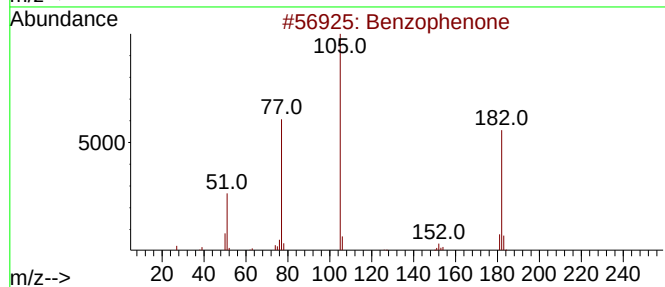
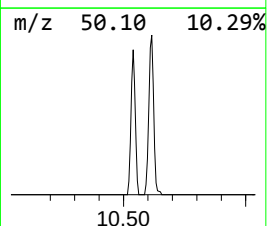
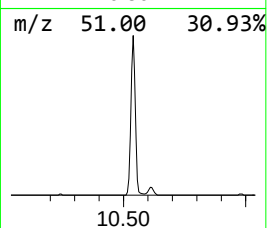
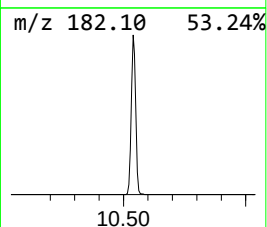
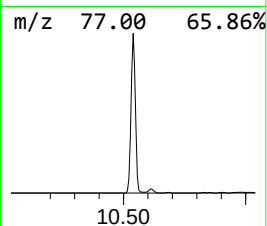
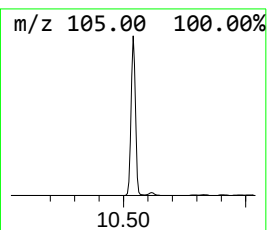
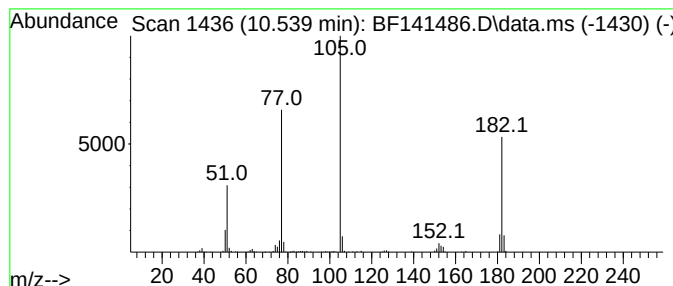
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.539	6.79 ng	311496	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	58
3			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50



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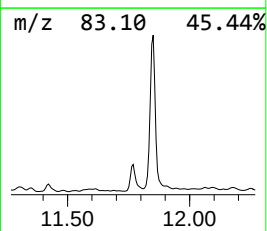
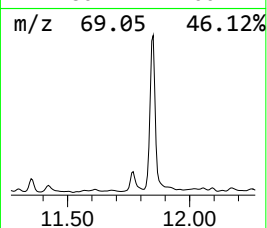
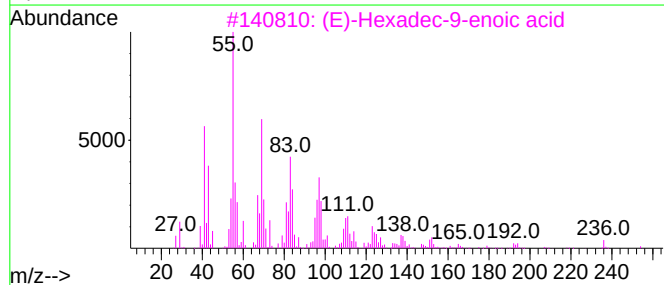
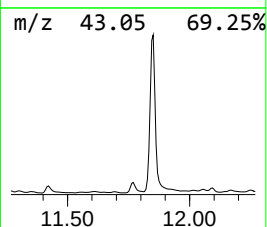
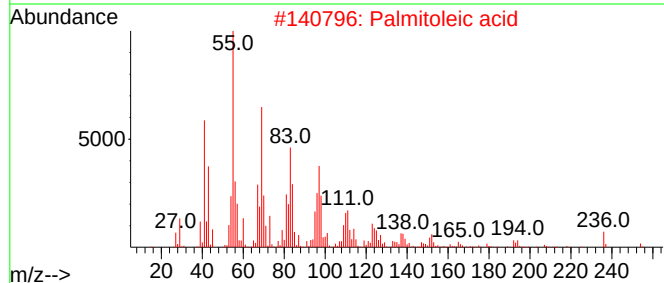
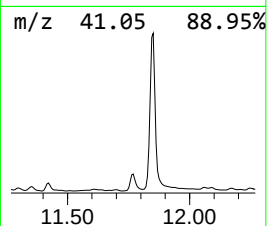
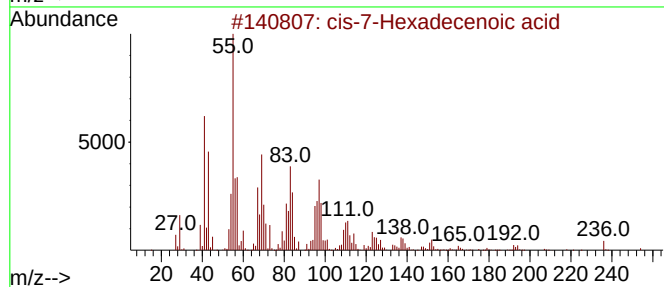
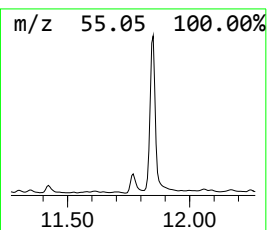
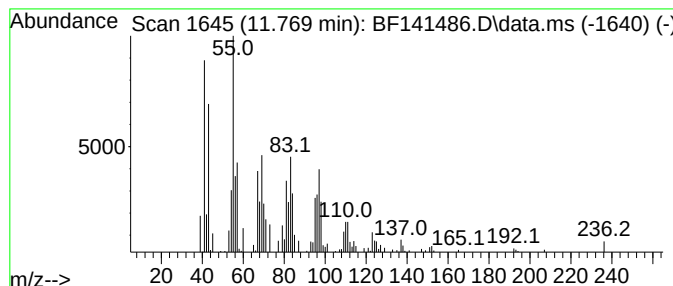
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Peak Number 3 cis-7-Hexadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	2.55 ng	122609	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	93
2			Palmitoleic acid	254	C16H30O2	000373-49-9	87
3			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	87
4			1,9-Tetradecadiene	194	C14H26	112929-06-3	83
5			Myristoleic acid	226	C14H26O2	000544-64-9	53



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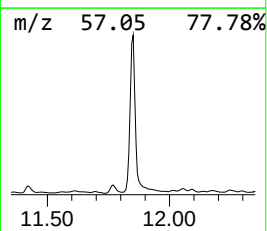
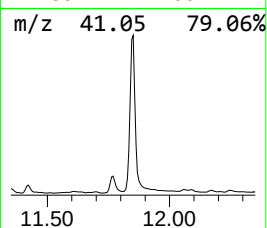
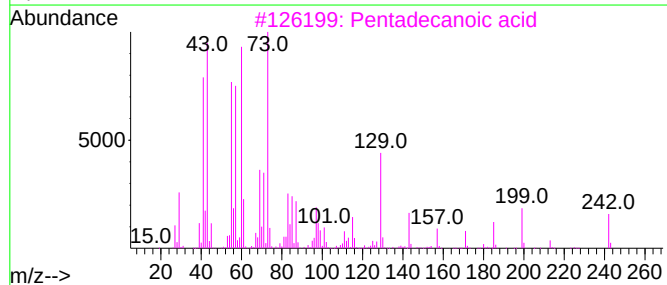
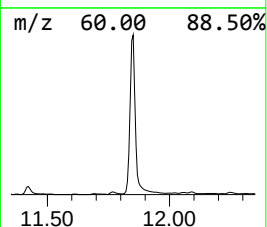
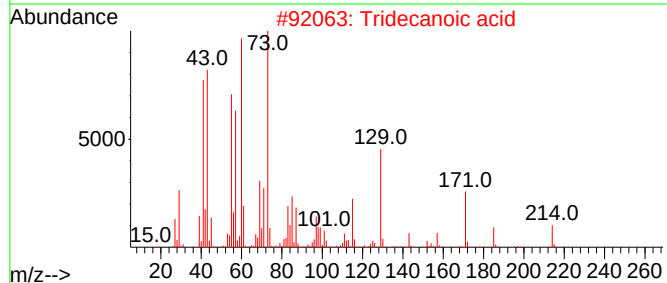
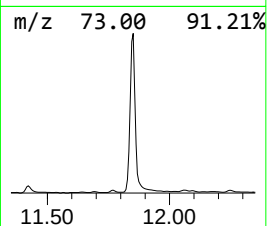
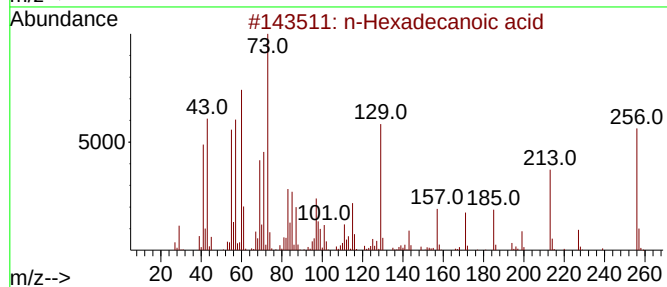
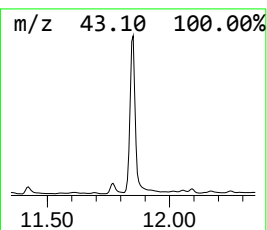
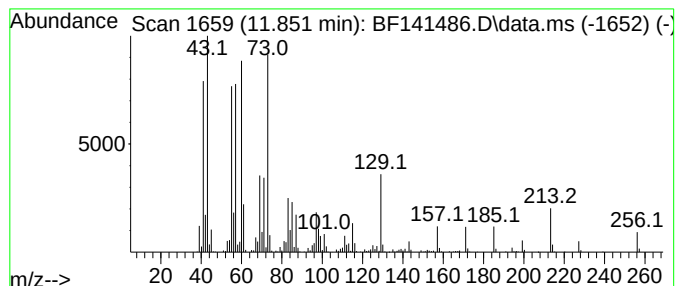
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.851	23.21 ng	1117770	Phenanthrene-d10	11.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



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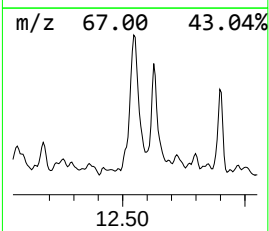
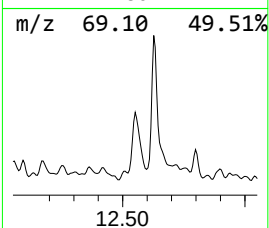
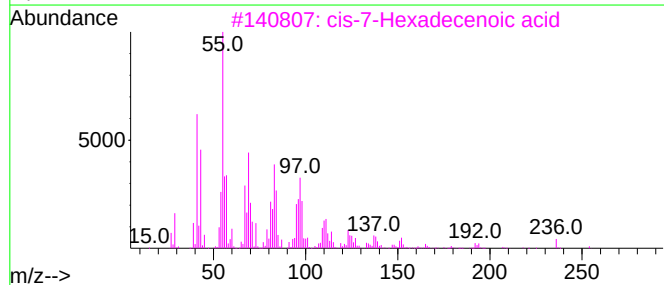
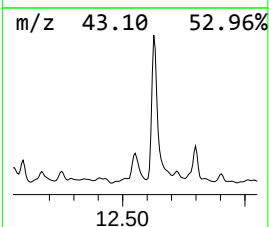
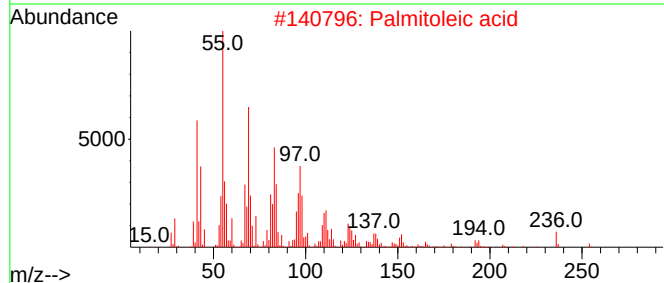
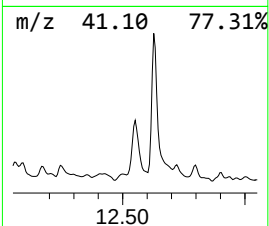
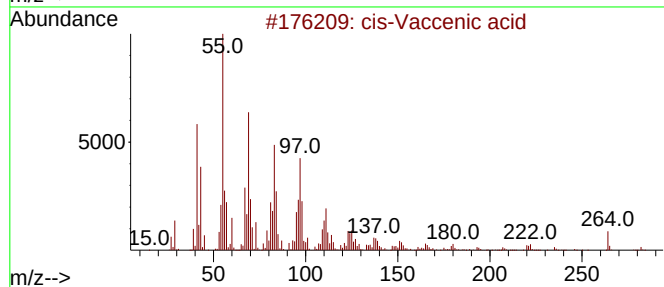
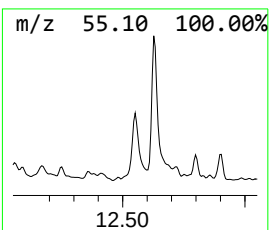
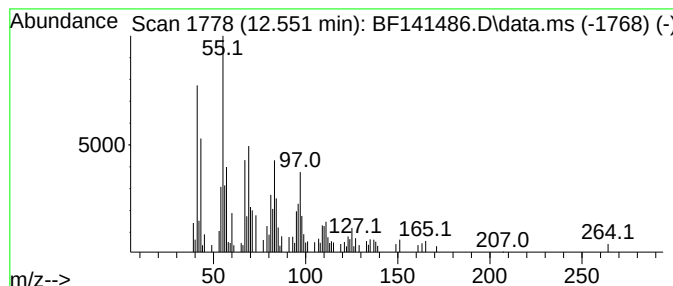
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Peak Number 5 cis-Vaccenic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	2.18 ng	105183	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
2			Palmitoleic acid	254	C16H30O2	000373-49-9	76
3			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	74
4			Oleic Acid	282	C18H34O2	000112-80-1	70
5			9-Hexadecenoic acid	254	C16H30O2	002091-29-4	68



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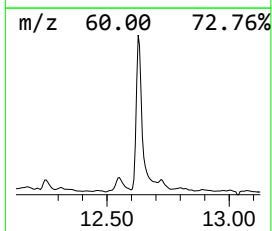
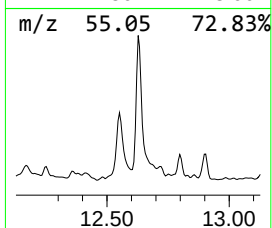
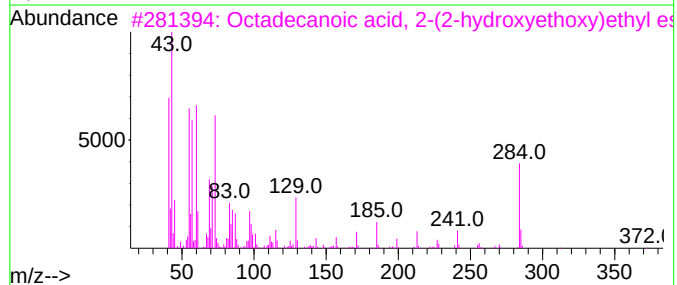
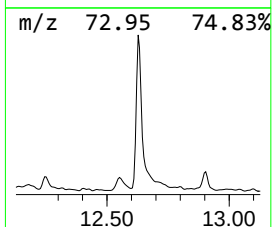
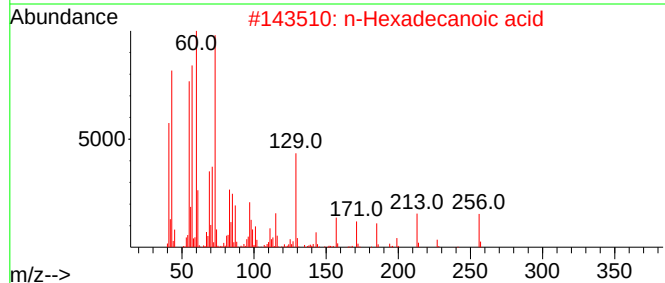
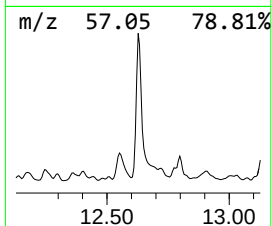
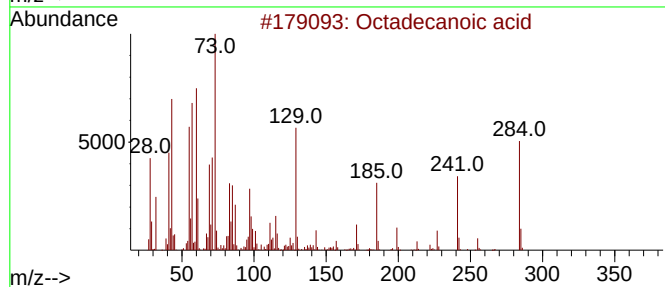
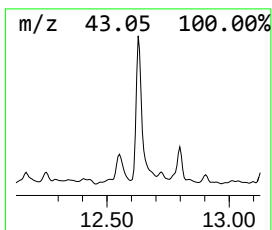
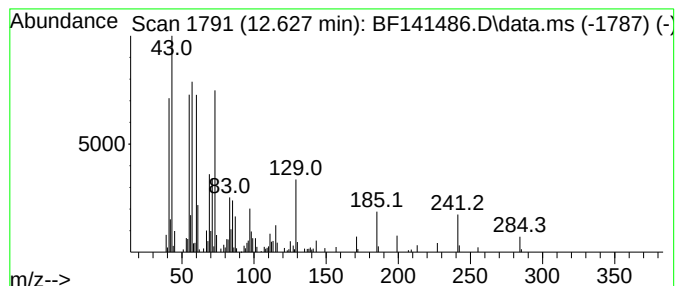
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	4.25 ng	204660	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020625\
Data File : BF141486.D
Acq On : 06 Feb 2025 18:00
Operator : RC/JU
Sample : Q1309-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

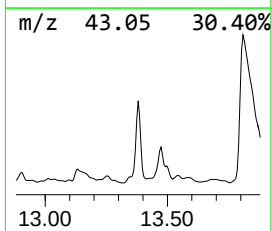
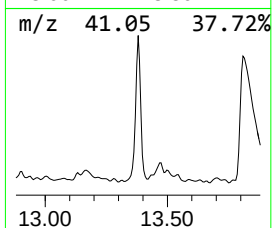
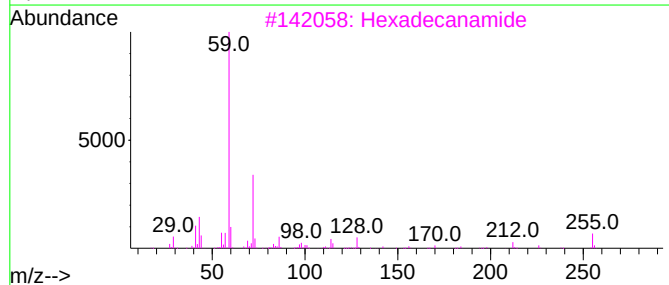
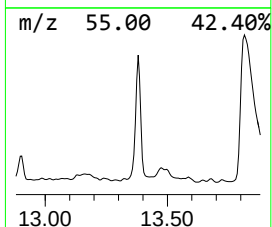
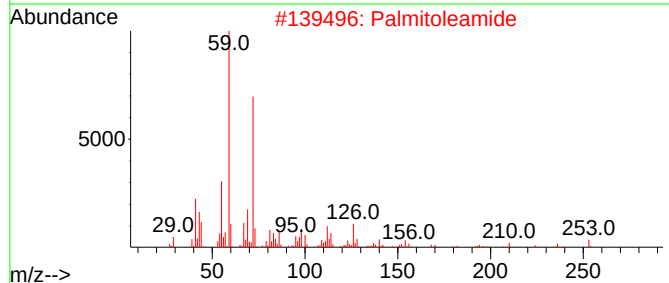
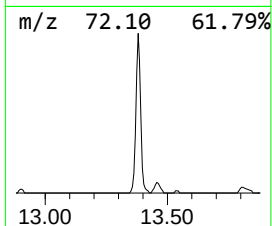
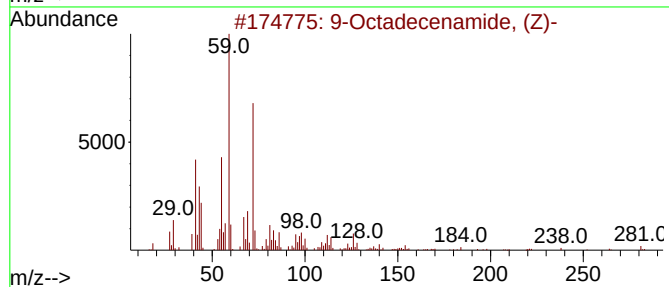
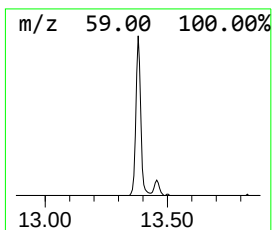
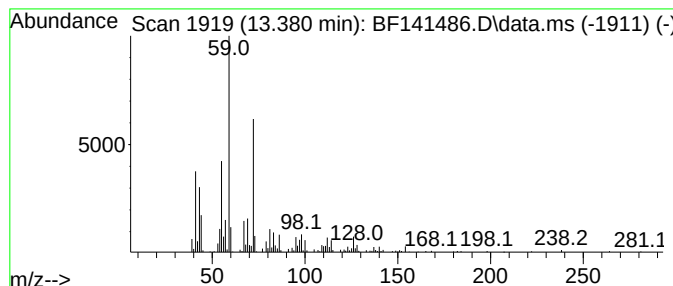
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.380	4.77 ng	181210	Chrysene-d12	13.951

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Palmitoleamide	253	C16H31NO	106010-22-4	90
3		Hexadecanamide	255	C16H33NO	000629-54-9	64
4		Octadecanamide	283	C18H37NO	000124-26-5	59
5		Octanamide	143	C8H17NO	000629-01-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020625\
Data File : BF141486.D
Acq On : 06 Feb 2025 18:00
Operator : RC/JU
Sample : Q1309-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

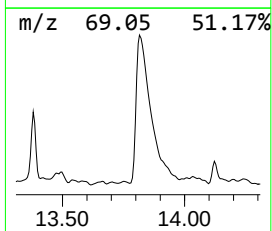
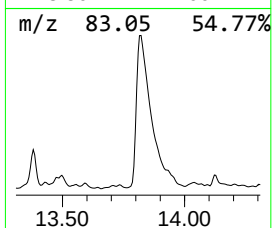
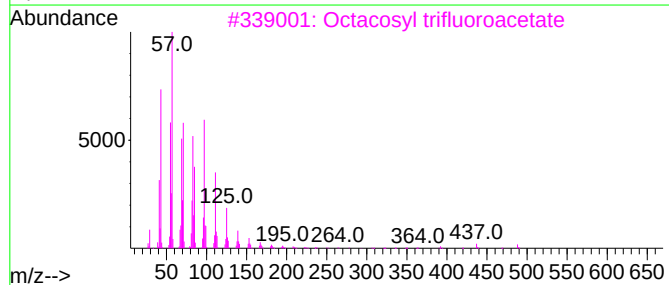
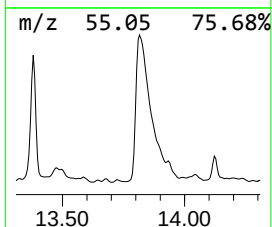
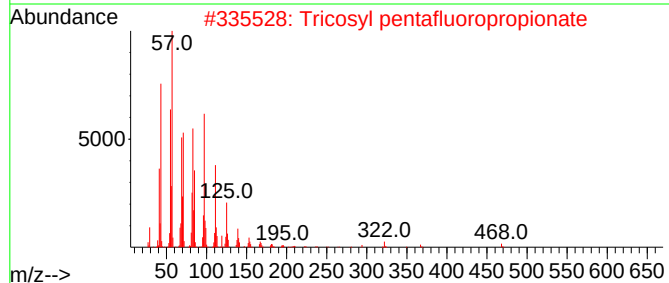
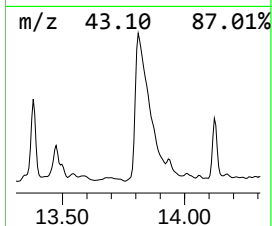
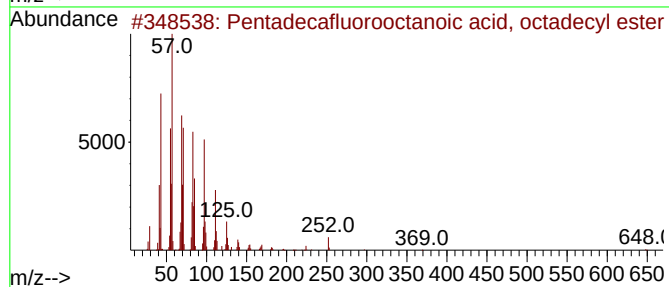
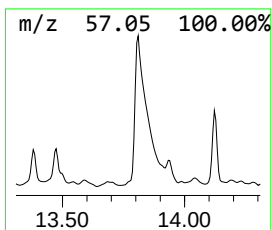
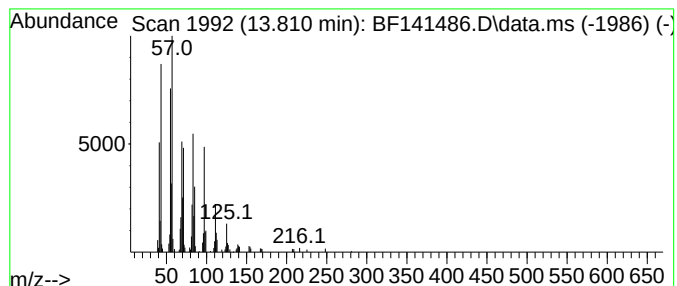
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.810	12.07 ng	459022	Chrysene-d12	13.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020625\
Data File : BF141486.D
Acq On : 06 Feb 2025 18:00
Operator : RC/JU
Sample : Q1309-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

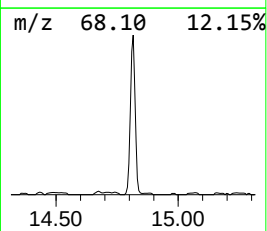
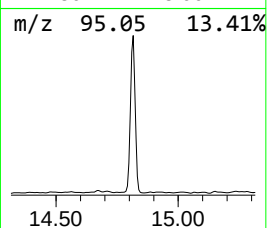
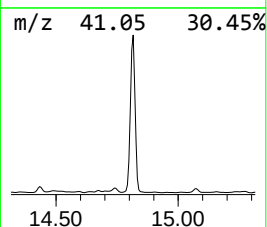
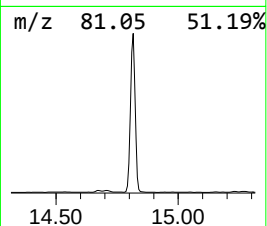
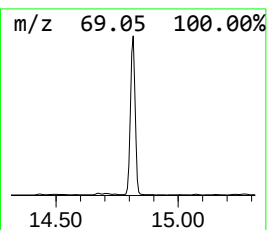
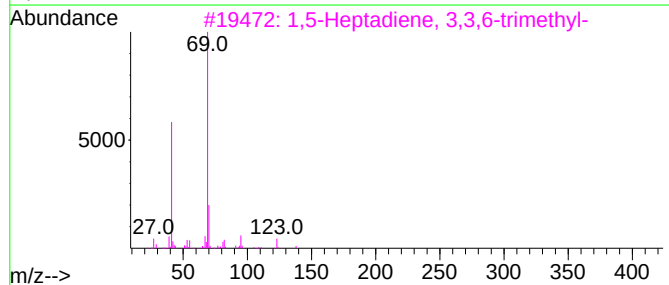
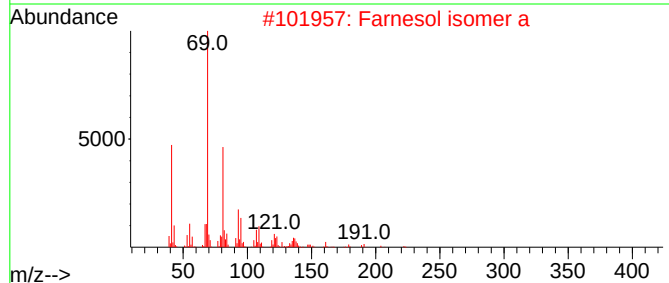
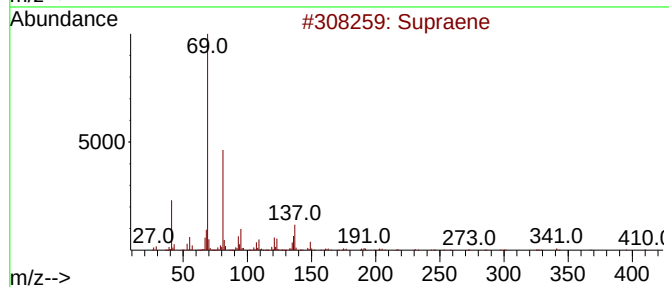
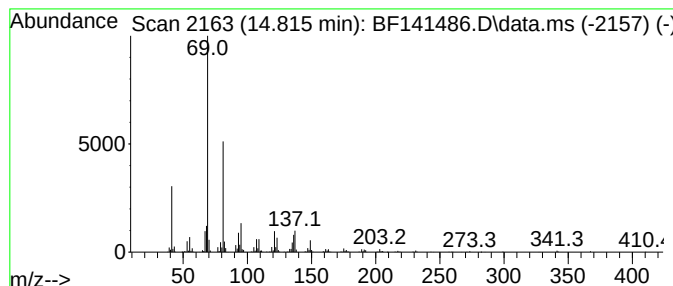
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	29.36 ng	859330	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Farnesol isomer a	222	C15H26O	1000108-92-4	64
3			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50
5			Squalene	410	C30H50	000111-02-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020625\
Data File : BF141486.D
Acq On : 06 Feb 2025 18:00
Operator : RC/JU
Sample : Q1309-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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
Pentanedioic ac...	7.604	2.3	ng	90444	2	8.069	778174	20.0
Benzophenone	10.539	6.8	ng	311496	3	9.822	917089	20.0
cis-7-Hexadecen...	11.769	2.5	ng	122609	4	11.310	963073	20.0
n-Hexadecanoic ...	11.851	23.2	ng	1117770	4	11.310	963073	20.0
cis-Vaccenic acid	12.551	2.2	ng	105183	4	11.310	963073	20.0
Octadecanoic acid	12.627	4.3	ng	204660	4	11.310	963073	20.0
9-Octadecenamid...	13.380	4.8	ng	181210	5	13.951	760421	20.0
Pentadecafluoro...	13.810	12.1	ng	459022	5	13.951	760421	20.0
Supraene	14.815	29.4	ng	859330	6	15.415	585399	20.0