

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072425\
 Data File : BF143235.D
 Acq On : 24 Jul 2025 15:58
 Operator : RC/JU
 Sample : Q2668-09
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF071725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.322	12	22	29	rVB	919576	1515965	58.40%	7.059%
2	4.116	320	327	335	rBV	25346	38776	1.49%	0.181%
3	5.199	504	511	519	rVB	204812	312834	12.05%	1.457%
4	5.593	571	578	584	rBV	1892364	2582442	99.48%	12.025%
5	6.581	740	746	752	rBV	1780712	2576375	99.25%	11.997%
6	6.957	805	810	816	rVB	533199	688721	26.53%	3.207%
7	7.351	872	877	888	rBV2	19047	27919	1.08%	0.130%
8	7.516	898	905	910	rBV	1295254	1729819	66.64%	8.055%
9	7.763	943	947	952	rBV	27600	32428	1.25%	0.151%
10	7.928	970	975	982	rBV2	11582	29471	1.14%	0.137%
11	8.239	1023	1028	1036	rBV	670028	837304	32.25%	3.899%
12	9.310	1205	1210	1216	rBV	1979606	2595923	100.00%	12.088%
13	9.992	1321	1326	1331	rBV	600152	748779	28.84%	3.487%
14	10.704	1442	1447	1454	rVB	286185	351945	13.56%	1.639%
15	10.781	1454	1460	1465	rBV	1030666	1289179	49.66%	6.003%
16	11.016	1495	1500	1504	rVB	44523	55889	2.15%	0.260%
17	11.480	1574	1579	1586	rBV	543130	700910	27.00%	3.264%
18	12.004	1661	1668	1680	rBV2	314286	521723	20.10%	2.429%
19	12.180	1694	1698	1703	rBV3	21083	34454	1.33%	0.160%
20	12.527	1750	1757	1771	rBV3	48997	131415	5.06%	0.612%
21	12.716	1781	1789	1797	rBV2	71823	249598	9.62%	1.162%
22	12.786	1797	1801	1808	rVV	62798	101726	3.92%	0.474%
23	12.922	1820	1824	1832	rVB	39849	65451	2.52%	0.305%
24	13.063	1843	1848	1853	rBV	1778636	2232505	86.00%	10.396%
25	13.963	1997	2001	2012	rVB	182073	324617	12.50%	1.512%
26	14.116	2022	2027	2035	rVB	569798	812162	31.29%	3.782%
27	14.980	2171	2174	2182	rVB	141509	201258	7.75%	0.937%
28	15.621	2279	2283	2295	rVB	380661	685460	26.41%	3.192%

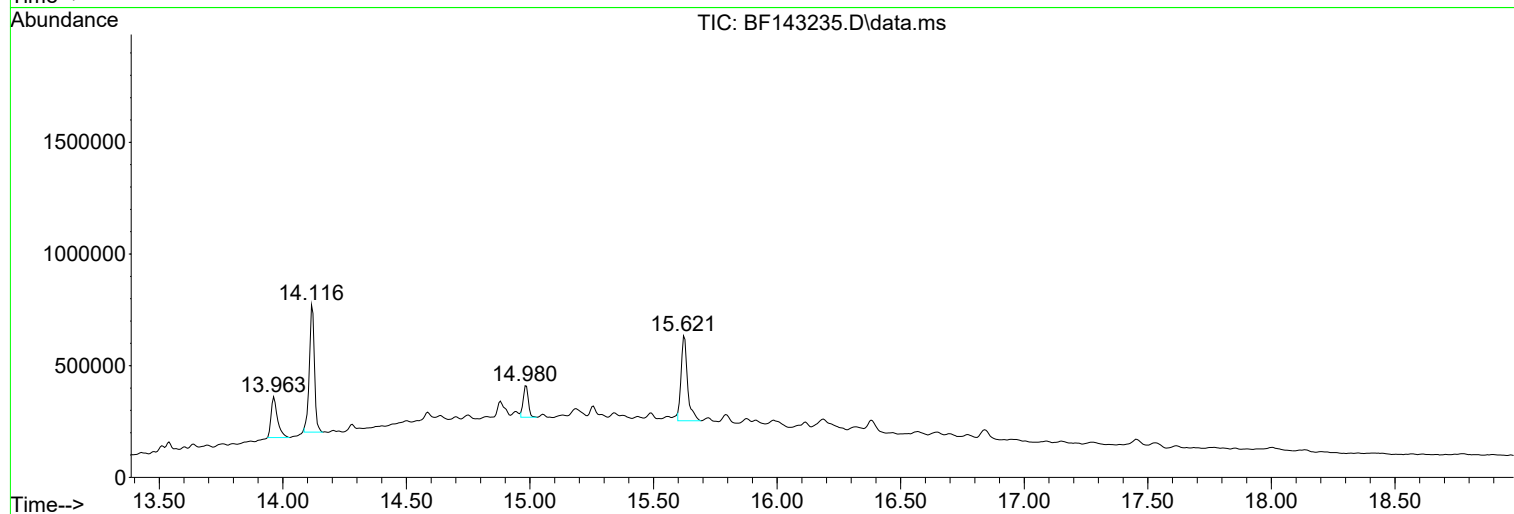
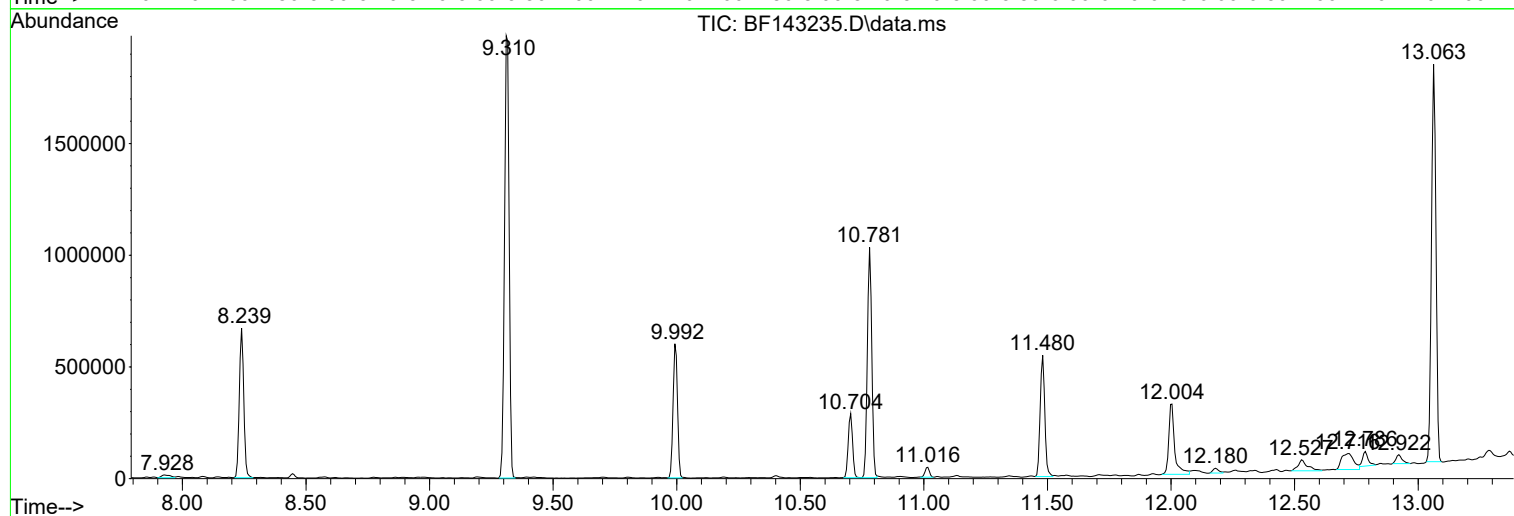
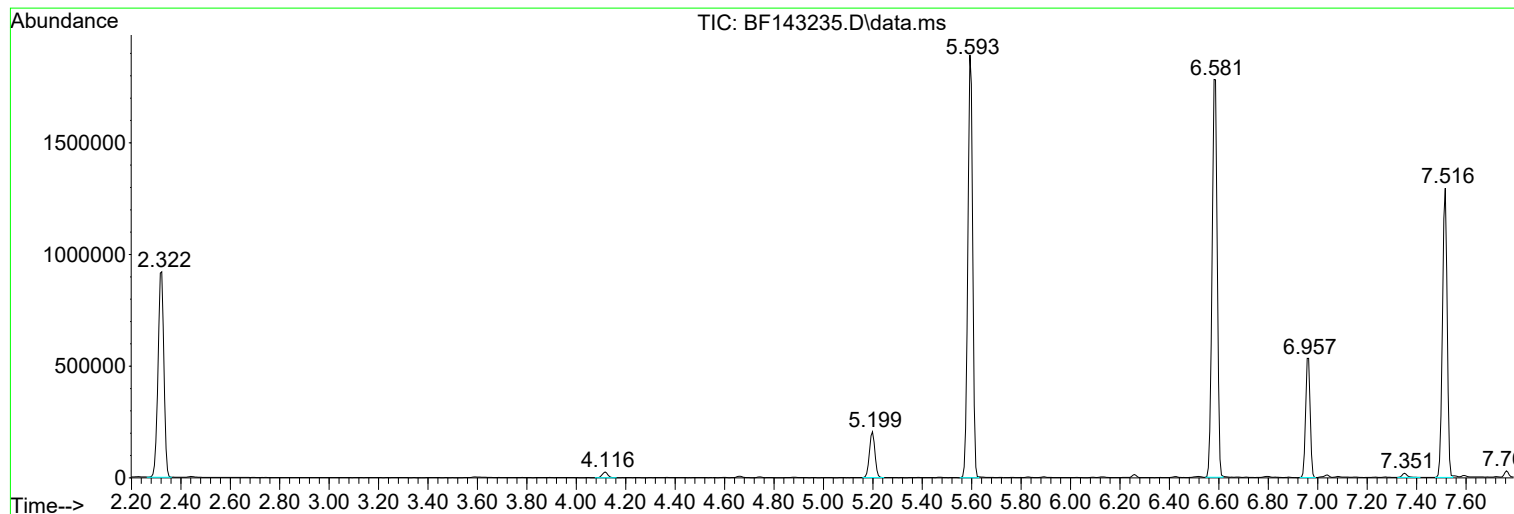
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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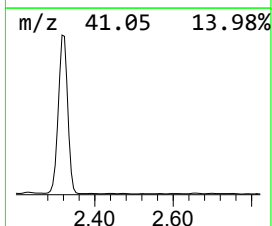
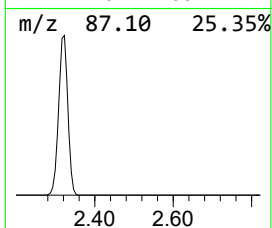
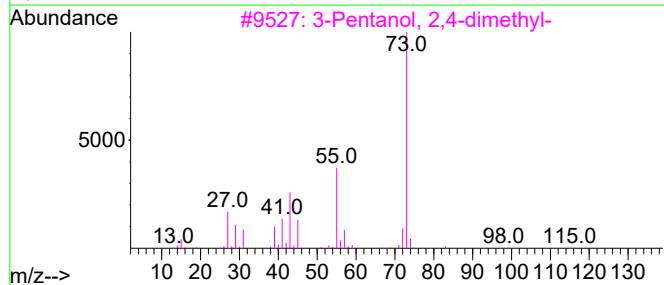
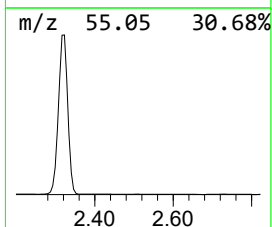
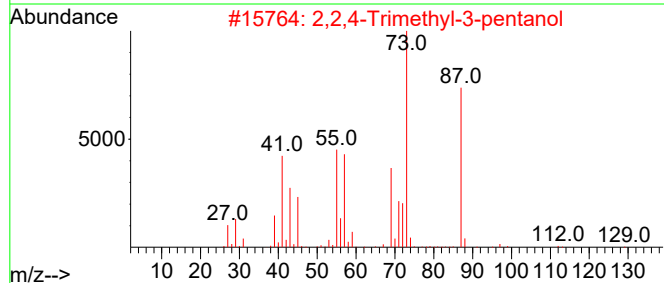
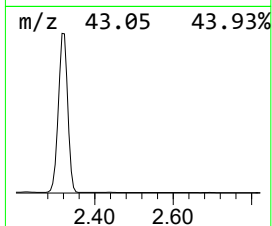
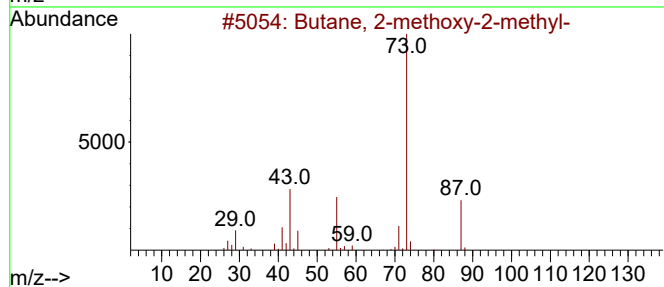
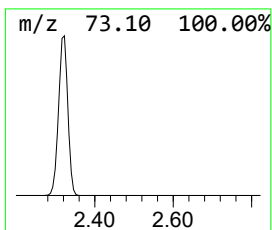
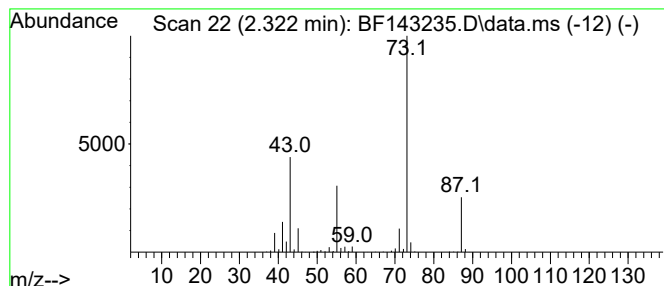
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	44.02 ng	1515970	1,4-Dichlorobenzene-d4	6.963

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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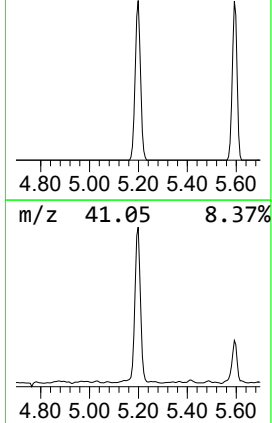
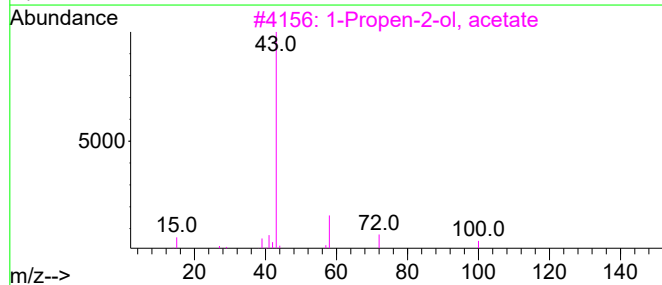
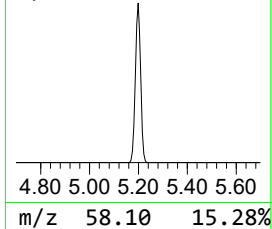
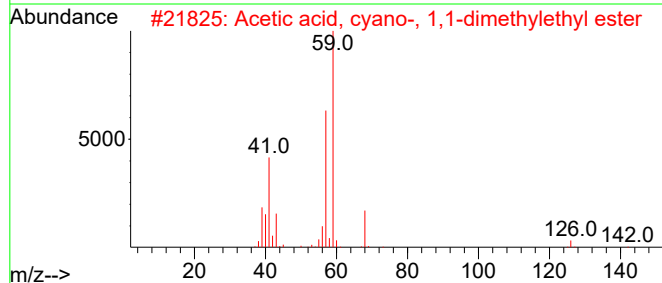
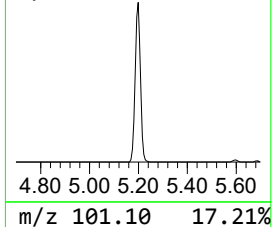
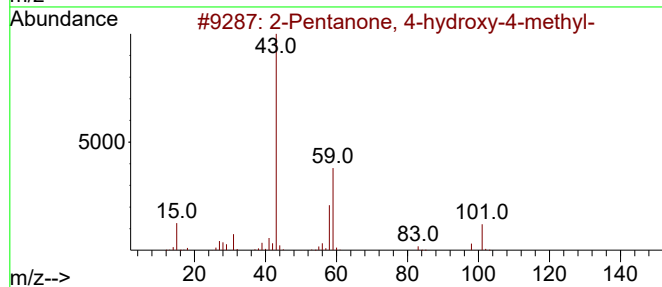
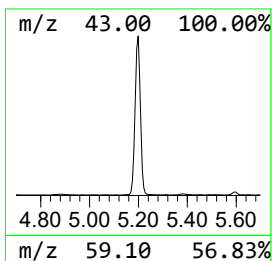
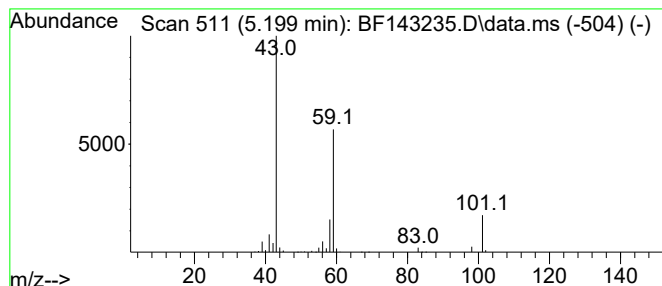
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.199	9.08 ng	312834	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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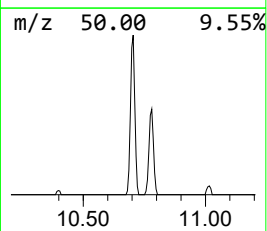
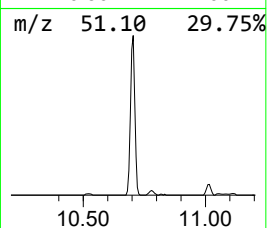
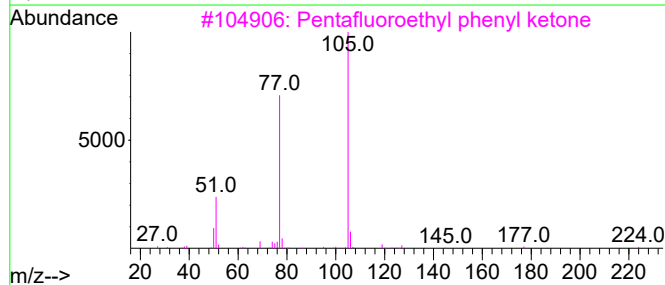
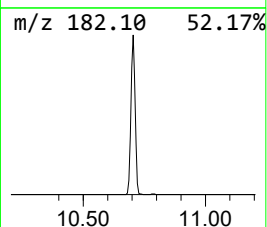
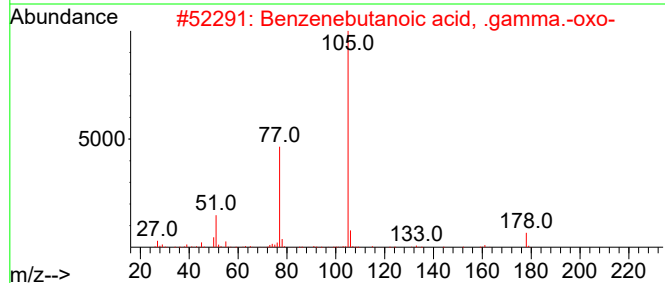
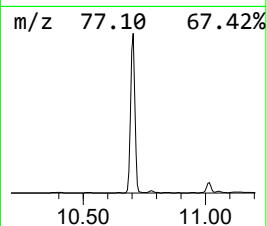
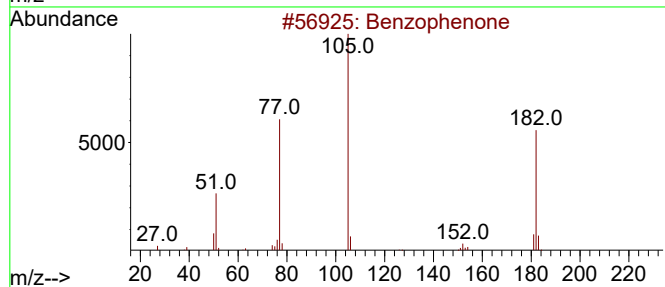
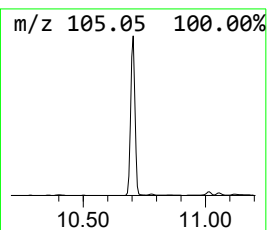
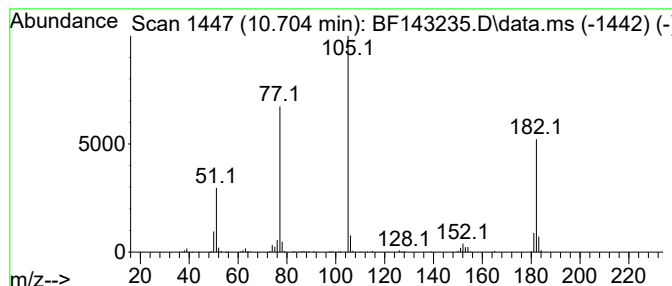
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.704	9.40 ng	351945	Acenaphthene-d10	9.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
3			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
4			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	50
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50



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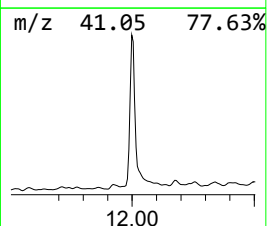
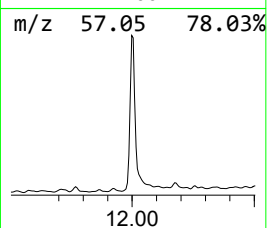
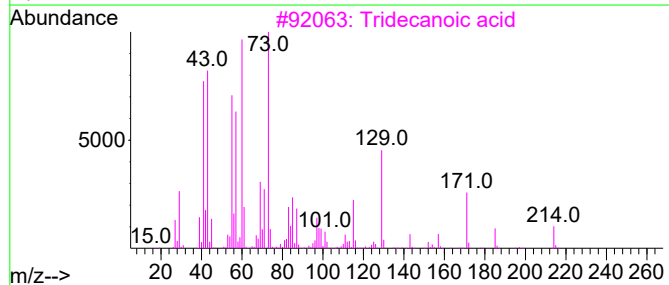
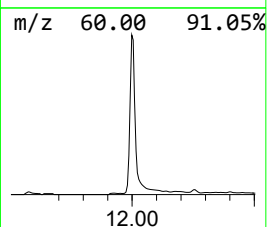
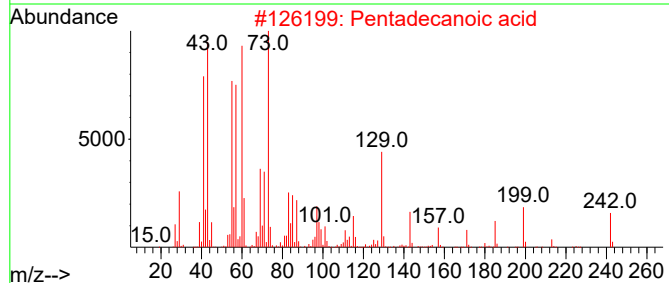
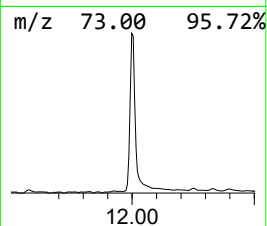
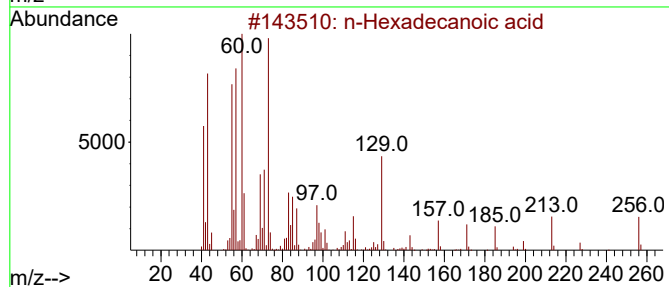
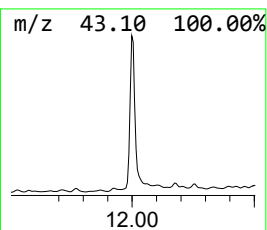
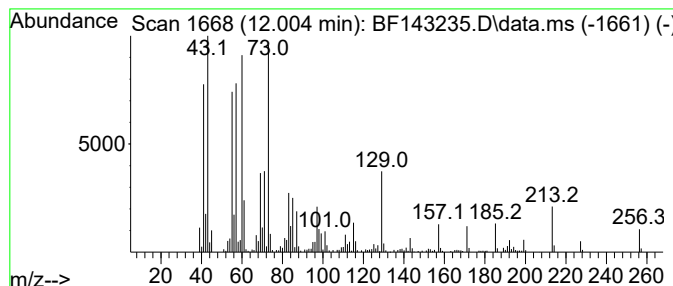
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	14.89 ng	521723	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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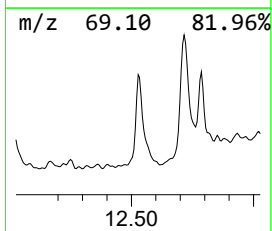
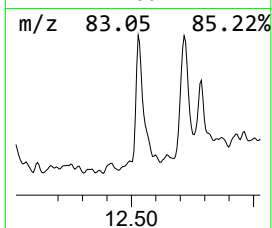
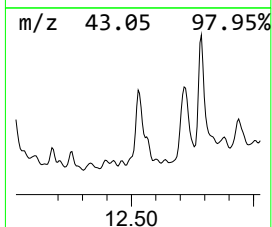
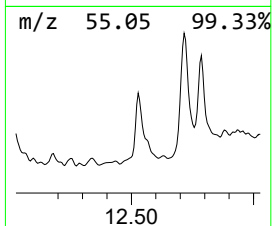
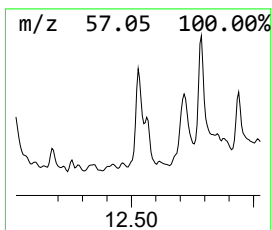
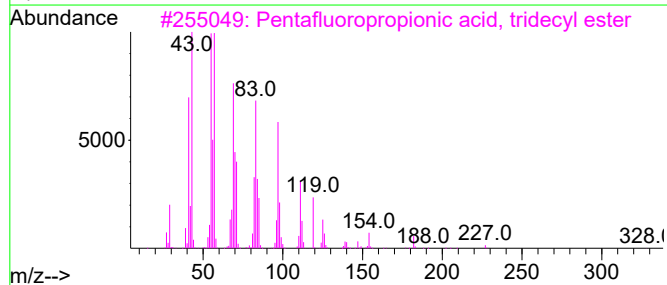
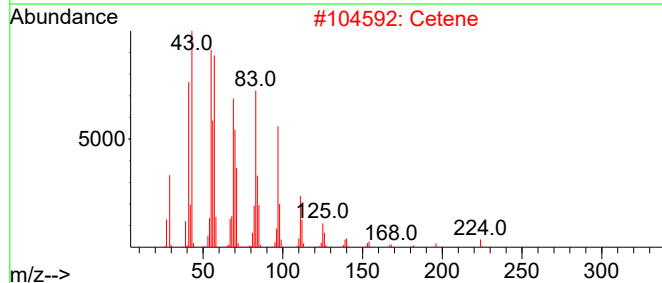
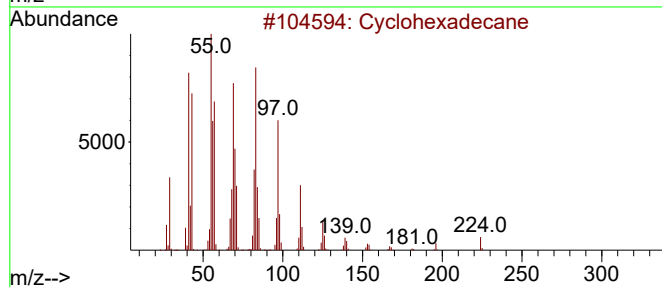
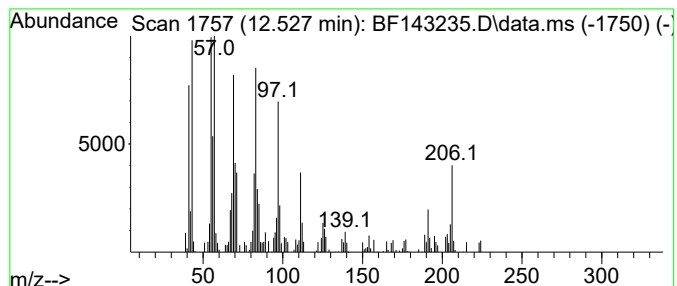
Instrument :
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Peak Number 5 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.528	3.75 ng	131415	Phenanthrene-d10		11.480	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexadecane		224	C16H32	000295-65-8	99
2	Cetene		224	C16H32	000629-73-2	94
3	Pentafluoropropionic acid, tridec...		346	C16H27F5O2	959261-22-4	93
4	n-Heptadecanol-1		256	C17H36O	001454-85-9	91
5	Bromoacetic acid, pentadecyl ester		348	C17H33BrO2	131143-01-6	91



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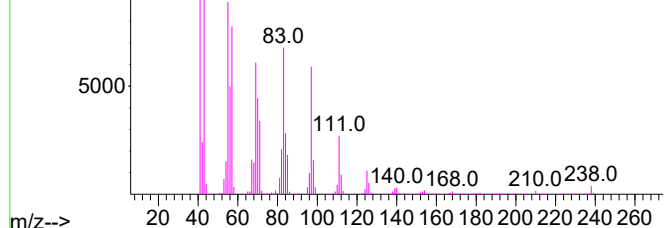
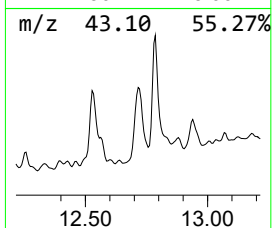
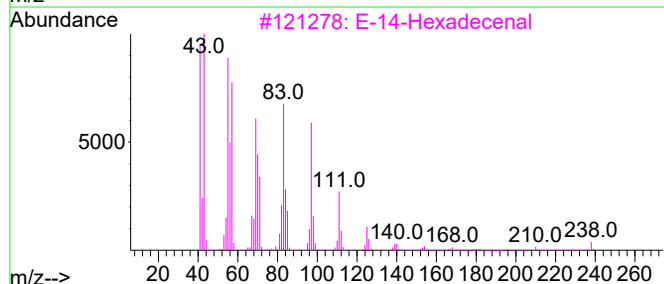
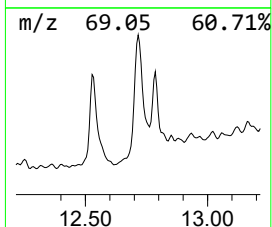
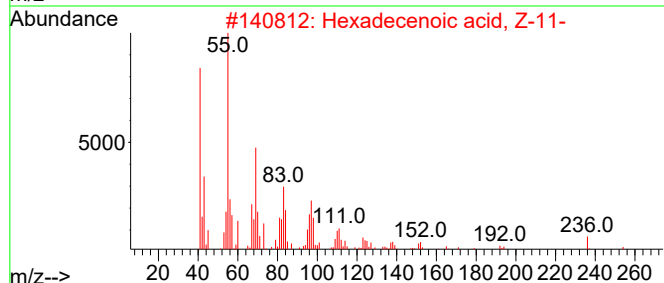
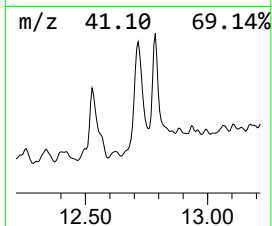
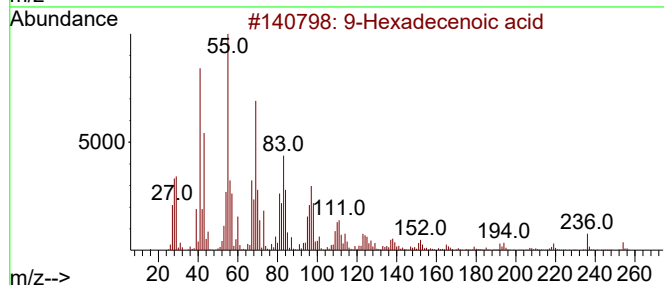
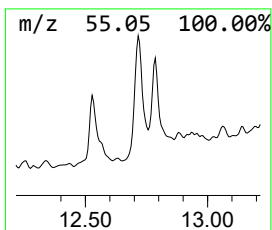
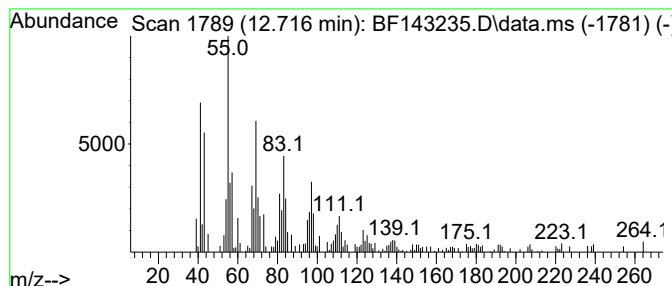
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Hexadecenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.716	7.12 ng	249598	Phenanthrene-d10		11.480	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid		254	C16H30O2	002091-29-4	95
2	Hexadecenoic acid, Z-11-		254	C16H30O2	002416-20-8	94
3	E-14-Hexadecenal		238	C16H30O	330207-53-9	93
4	Oxacycloheptadecan-2-one		254	C16H30O2	000109-29-5	89
5	Oleic Acid		282	C18H34O2	000112-80-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072425\
Data File : BF143235.D
Acq On : 24 Jul 2025 15:58
Operator : RC/JU
Sample : Q2668-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

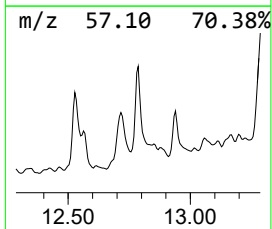
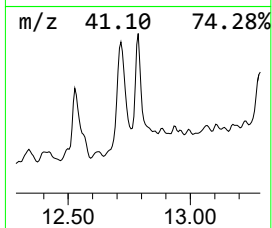
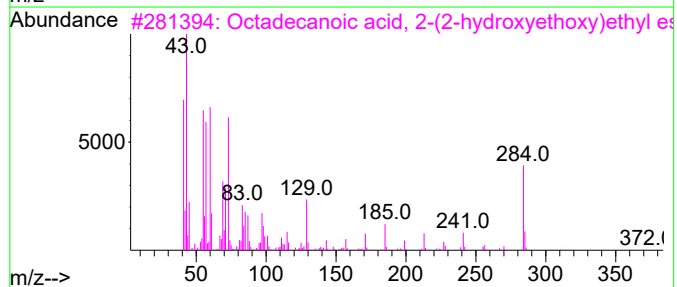
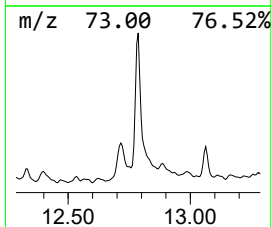
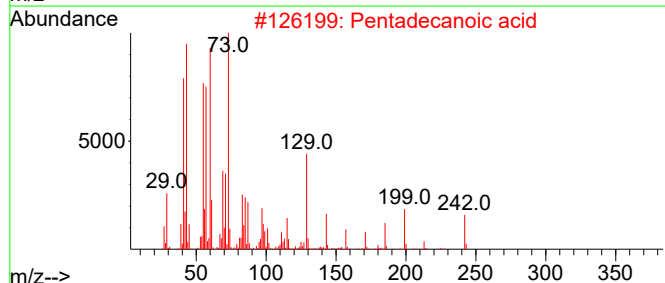
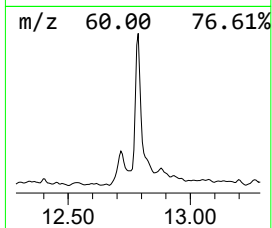
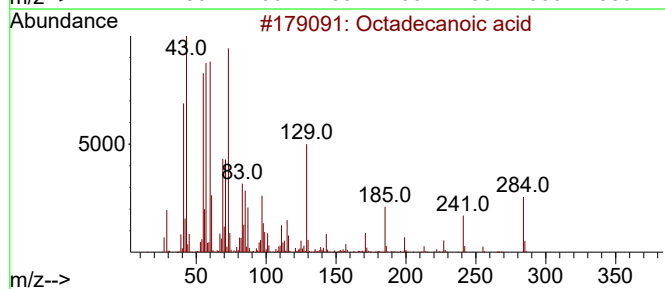
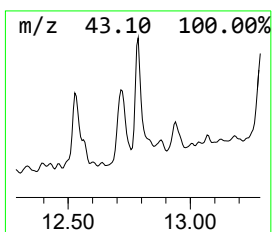
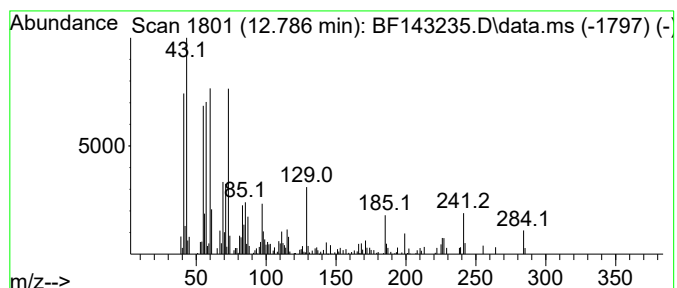
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.786	2.90 ng	101726	Phenanthrene-d10		11.480	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	83
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	81
5	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072425\
Data File : BF143235.D
Acq On : 24 Jul 2025 15:58
Operator : RC/JU
Sample : Q2668-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

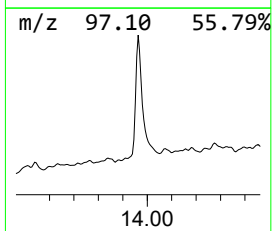
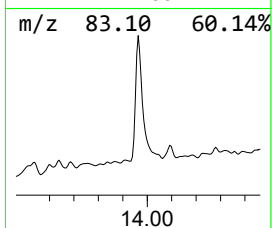
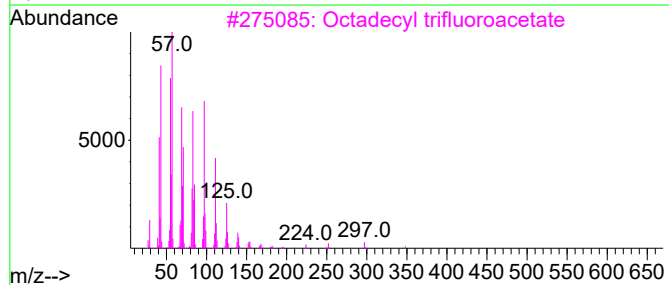
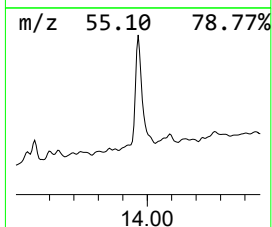
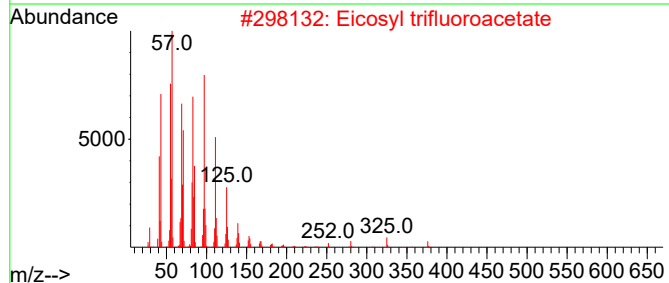
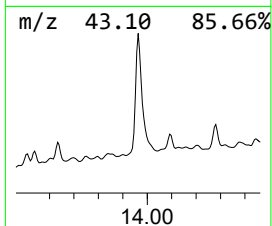
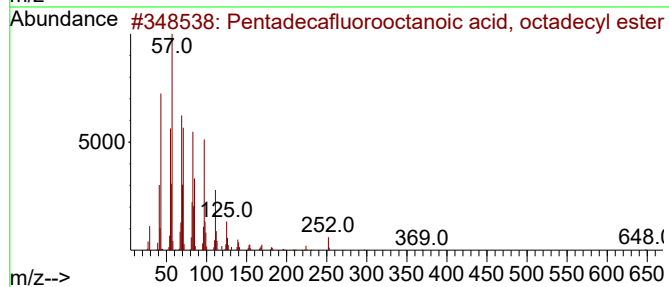
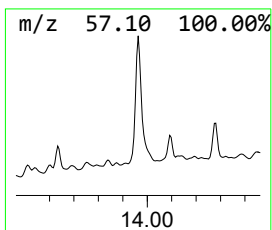
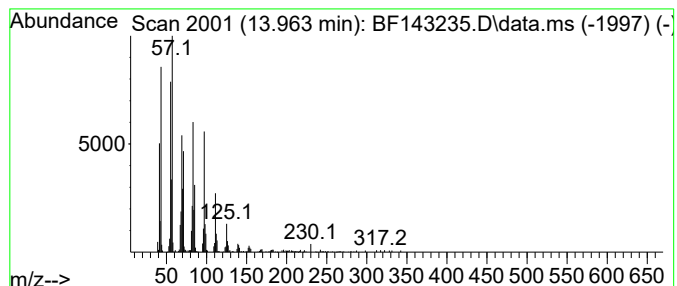
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.963	7.99 ng	324617	Chrysene-d12	14.116	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072425\
Data File : BF143235.D
Acq On : 24 Jul 2025 15:58
Operator : RC/JU
Sample : Q2668-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

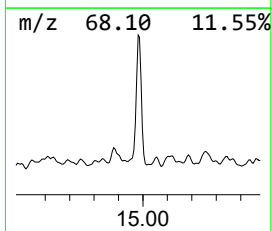
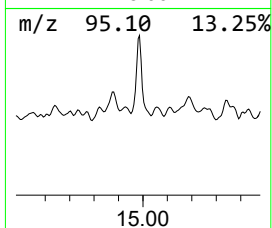
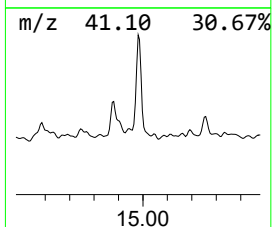
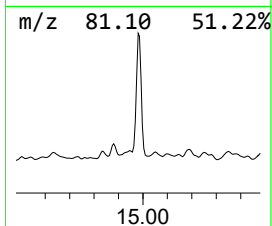
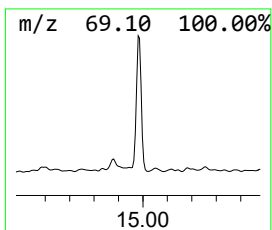
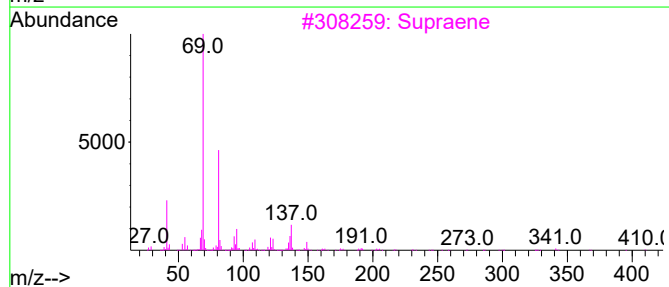
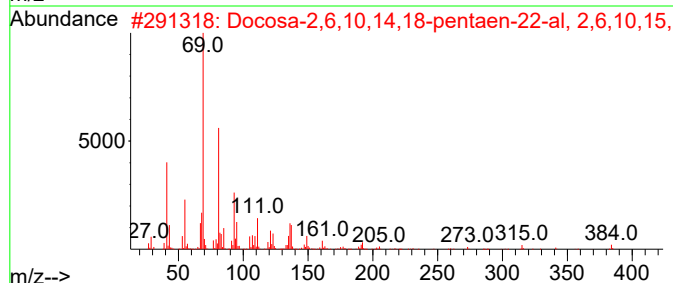
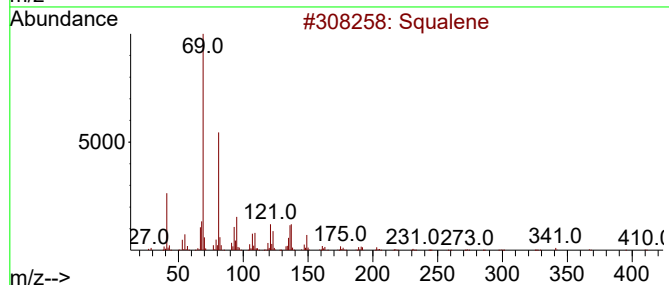
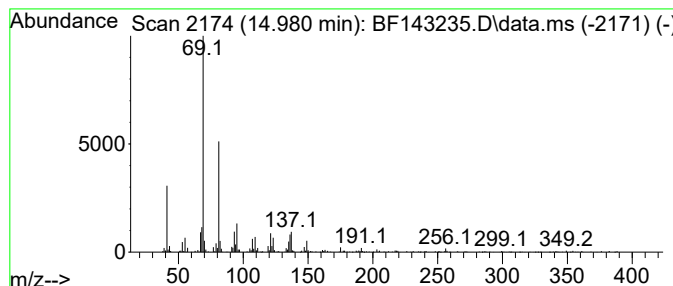
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	5.87 ng	201258	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3			Supraene	410	C30H50	007683-64-9	83
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072425\
Data File : BF143235.D
Acq On : 24 Jul 2025 15:58
Operator : RC/JU
Sample : Q2668-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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...	2.322	44.0	ng	1515970	1	6.963	688721	20.0
2-Pentanone, 4-...	5.199	9.1	ng	312834	1	6.963	688721	20.0
Benzophenone	10.704	9.4	ng	351945	3	9.992	748779	20.0
n-Hexadecanoic ...	12.004	14.9	ng	521723	4	11.480	700910	20.0
Cyclohexadecane	12.528	3.8	ng	131415	4	11.480	700910	20.0
9-Hexadecenoic ...	12.716	7.1	ng	249598	4	11.480	700910	20.0
Octadecanoic acid	12.786	2.9	ng	101726	4	11.480	700910	20.0
Pentadecafluoro...	13.963	8.0	ng	324617	5	14.116	812162	20.0
Squalene	14.980	5.9	ng	201258	6	15.621	685460	20.0