

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072325\
 Data File : BF143217.D
 Acq On : 23 Jul 2025 17:57
 Operator : RC/JU
 Sample : Q2649-05
 Misc :
 ALS Vial : 9 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-BF071725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143217.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	13	21	28	rVB	822184	1312773	37.57%	4.699%
2	5.198	503	511	525	rBV	267637	411515	11.78%	1.473%
3	5.598	573	579	584	rBV	2176751	2951319	84.45%	10.565%
4	6.587	740	747	753	rBV	2328644	3434632	98.28%	12.295%
5	6.963	805	811	816	rVB	627357	775082	22.18%	2.774%
6	7.516	898	905	910	rBV	1467853	1959270	56.07%	7.013%
7	7.763	943	947	952	rBV	39683	47575	1.36%	0.170%
8	8.239	1023	1028	1037	rBV	808880	1054004	30.16%	3.773%
9	8.445	1057	1063	1068	rBV	34943	45773	1.31%	0.164%
10	9.316	1205	1211	1216	rBV	2577070	3260907	93.31%	11.673%
11	9.998	1322	1327	1332	rVB	898220	1132961	32.42%	4.056%
12	10.704	1442	1447	1455	rVB	520768	662032	18.94%	2.370%
13	10.786	1455	1461	1466	rBV	1771489	2351398	67.29%	8.417%
14	11.016	1496	1500	1504	rVB	76751	92729	2.65%	0.332%
15	11.139	1515	1521	1531	rBV	97753	138709	3.97%	0.497%
16	11.480	1572	1579	1584	rBV	898506	1128581	32.29%	4.040%
17	11.574	1591	1595	1604	rBV2	36082	53076	1.52%	0.190%
18	11.927	1649	1655	1661	rBV	125317	186933	5.35%	0.669%
19	12.004	1663	1668	1684	rVV	663209	945187	27.05%	3.383%
20	12.504	1749	1753	1761	rVB2	22507	35798	1.02%	0.128%
21	12.710	1781	1788	1796	rBV2	53506	108491	3.10%	0.388%
22	12.786	1796	1801	1813	rVV	116670	175681	5.03%	0.629%
23	13.068	1843	1849	1854	rBV	2675752	3494622	100.00%	12.509%
24	13.963	1995	2001	2015	rBV	131527	248924	7.12%	0.891%
25	14.115	2022	2027	2033	rBV	549515	719076	20.58%	2.574%
26	14.280	2051	2055	2061	rBV	29223	43568	1.25%	0.156%
27	14.586	2103	2107	2115	rBV	29626	49181	1.41%	0.176%
28	14.980	2169	2174	2180	rBV	281708	384157	10.99%	1.375%
29	15.621	2277	2283	2295	rBV	464136	732229	20.95%	2.621%

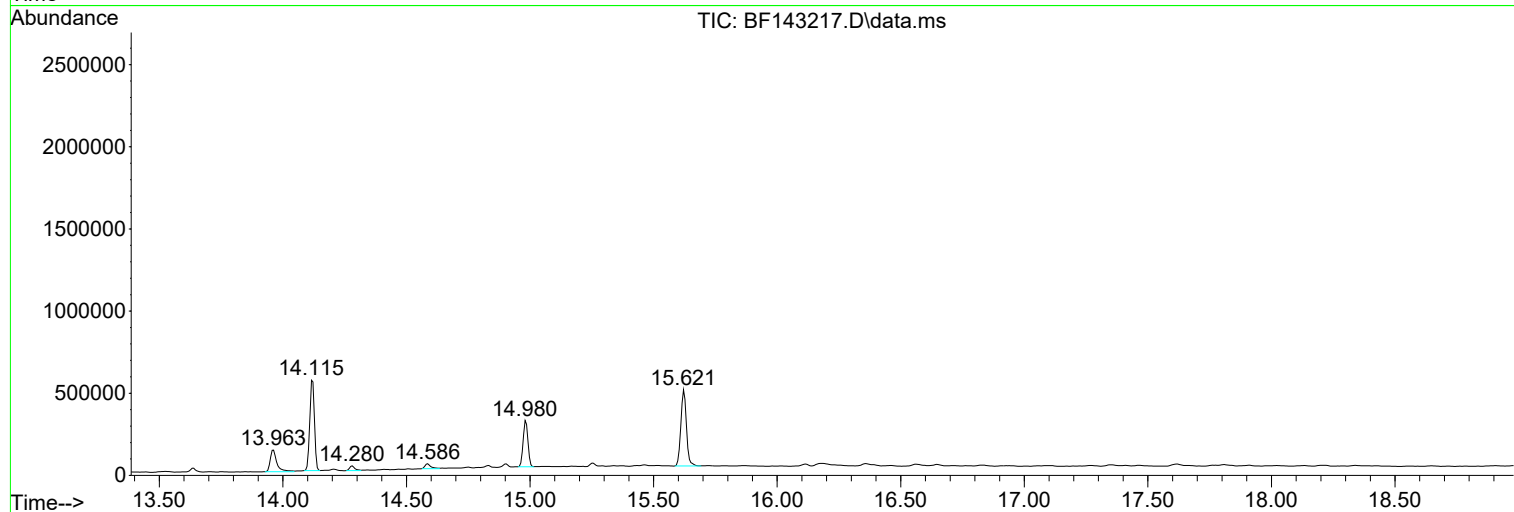
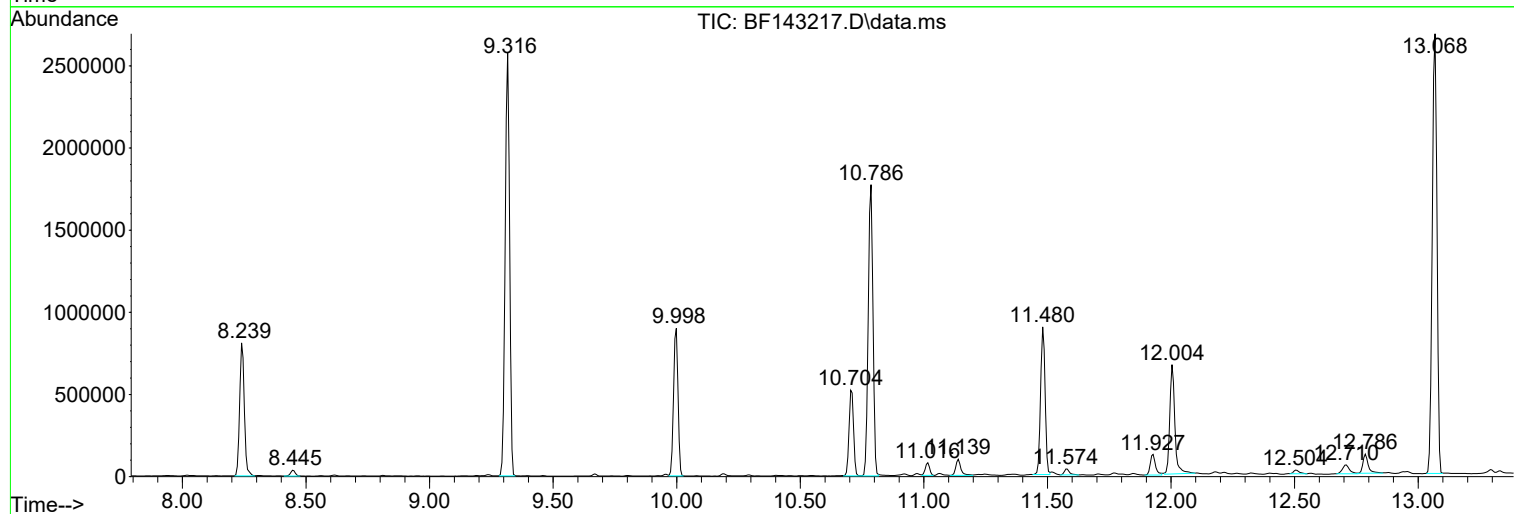
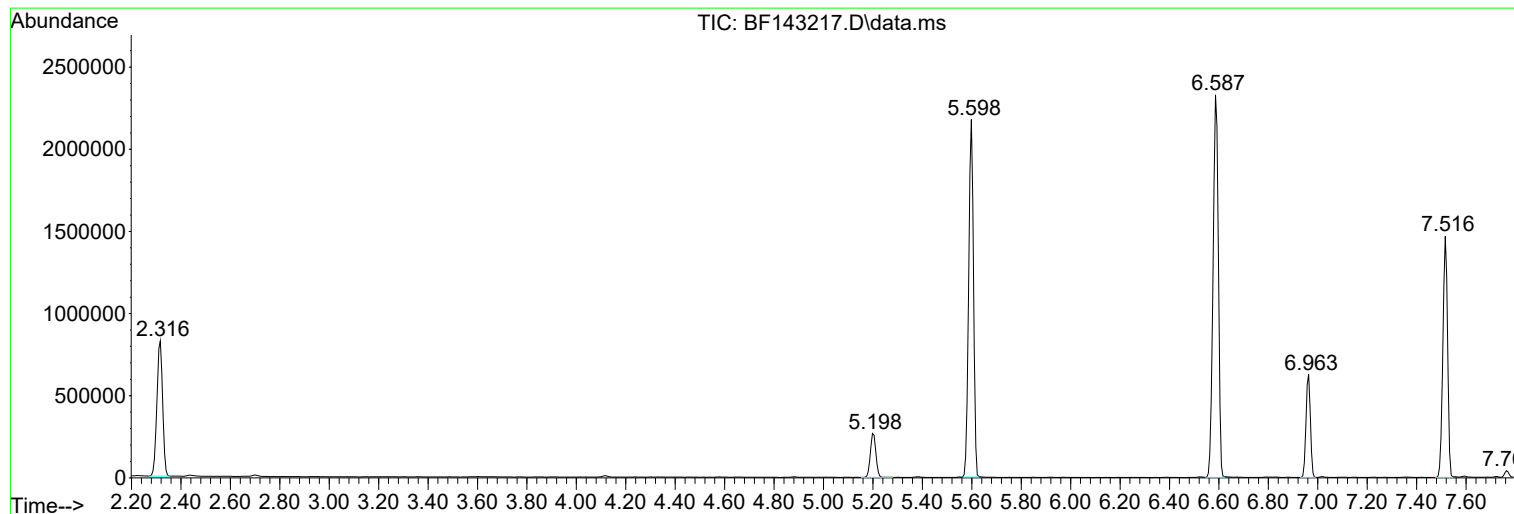
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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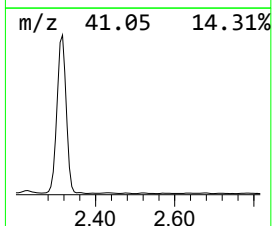
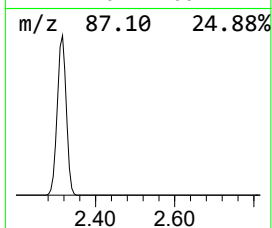
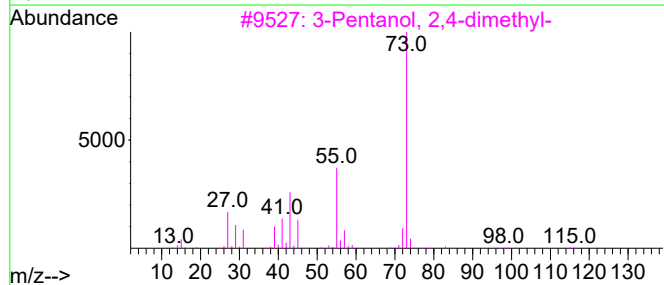
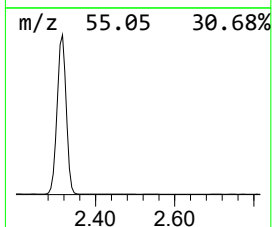
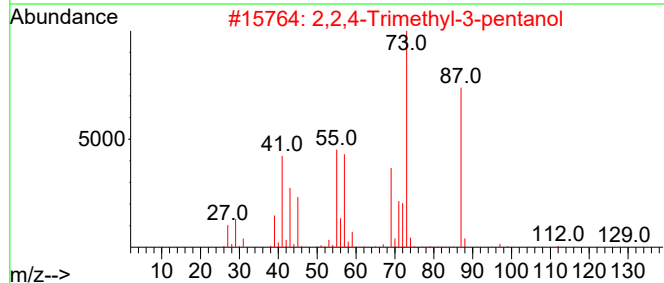
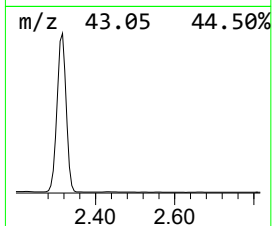
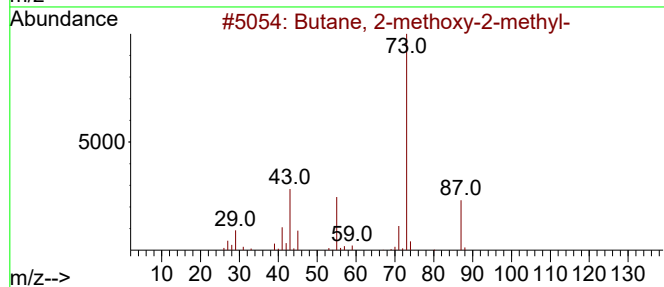
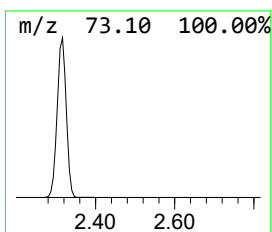
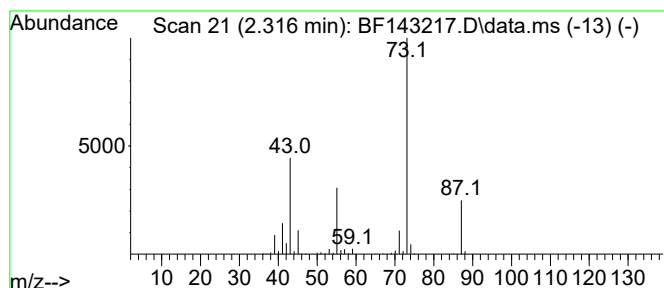
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.316	33.87 ng	1312770	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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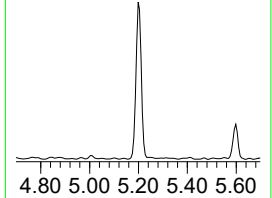
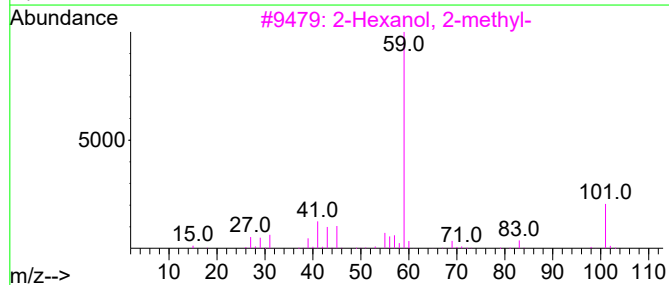
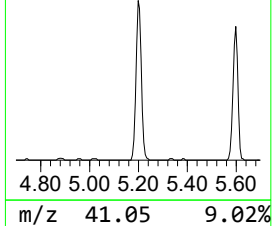
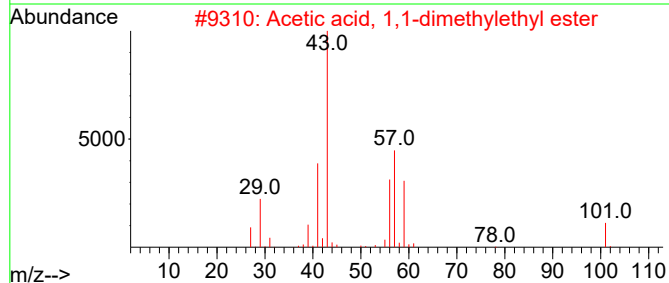
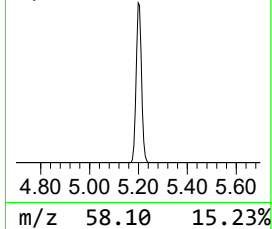
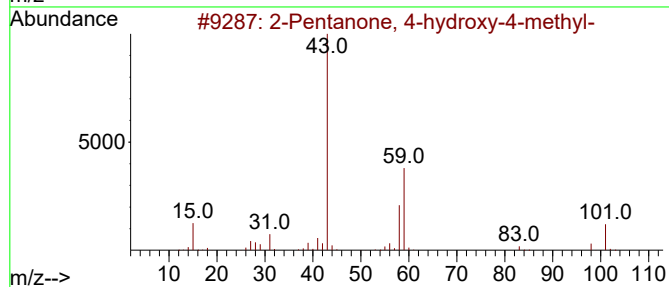
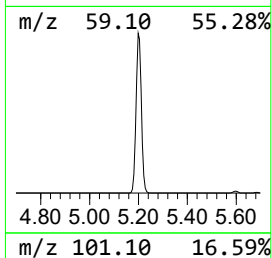
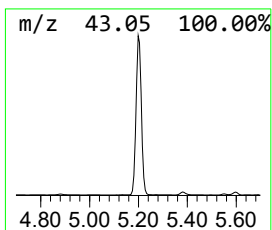
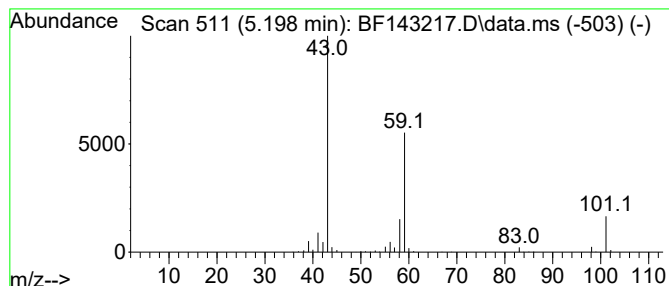
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	10.62 ng	411515	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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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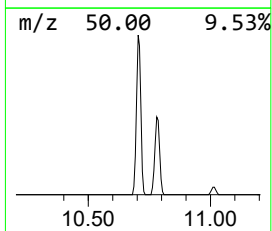
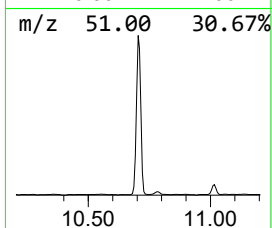
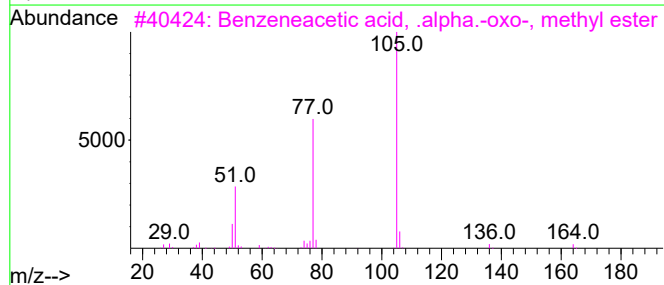
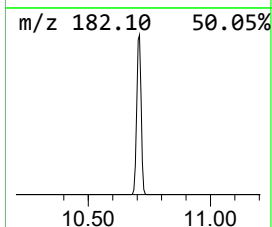
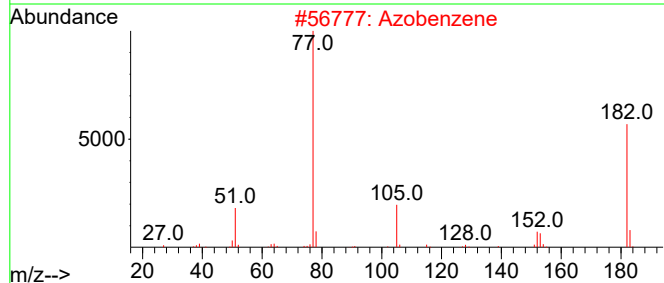
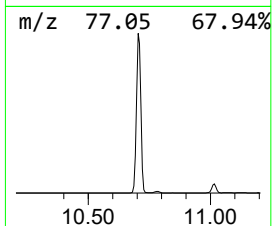
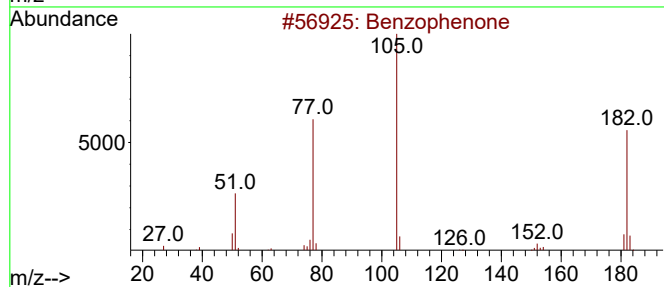
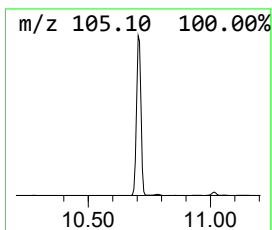
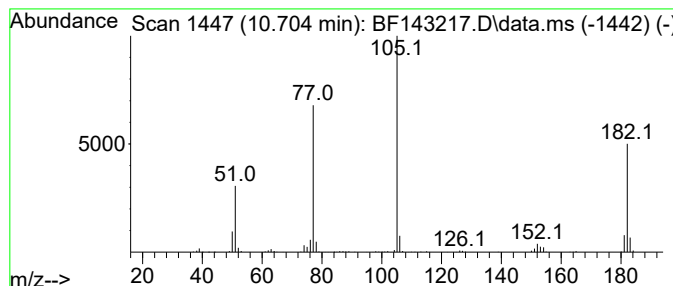
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.704	11.69 ng	662032	Acenaphthene-d10	9.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	58
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50



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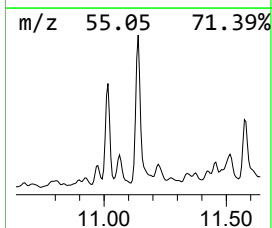
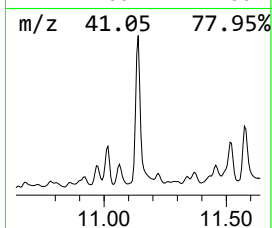
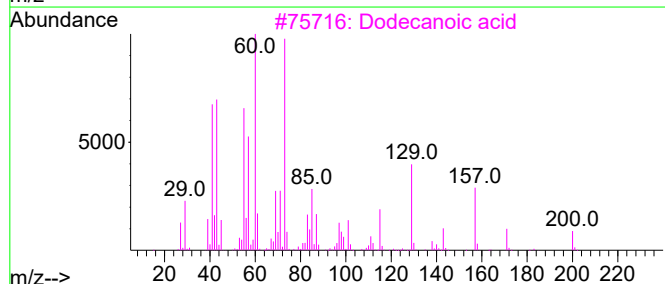
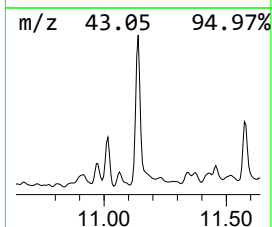
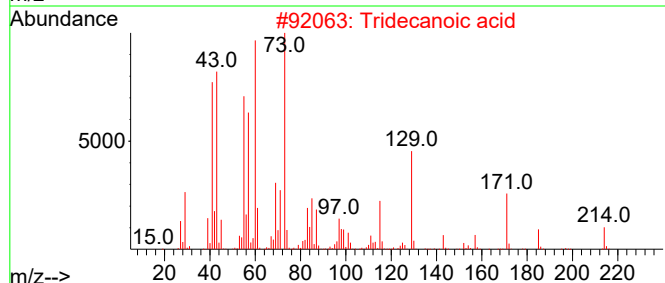
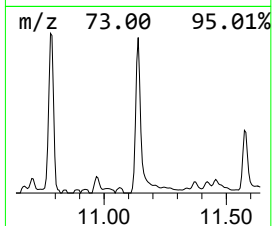
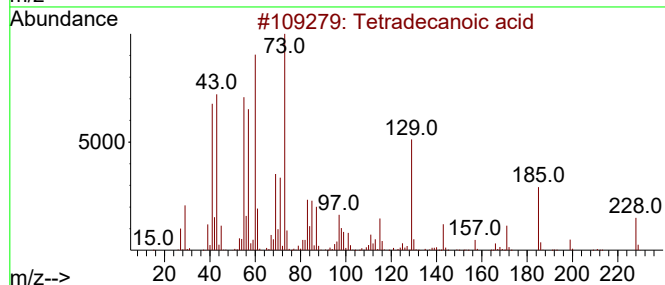
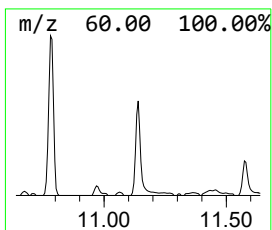
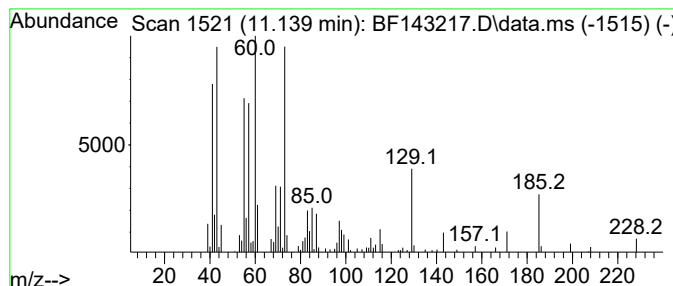
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.139	2.46 ng	138709	Phenanthrene-d10		11.480	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
2	Tridecanoic acid		214	C13H26O2	000638-53-9	80
3	Dodecanoic acid		200	C12H24O2	000143-07-7	64
4	n-Decanoic acid		172	C10H20O2	000334-48-5	53
5	Undecanoic acid		186	C11H22O2	000112-37-8	50



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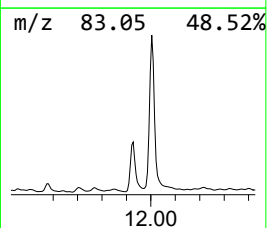
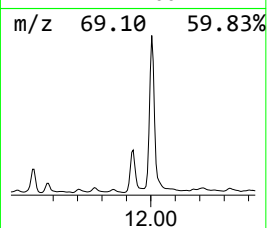
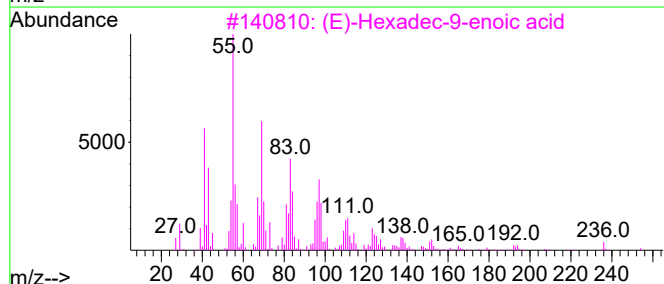
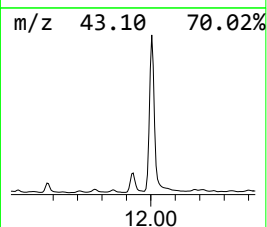
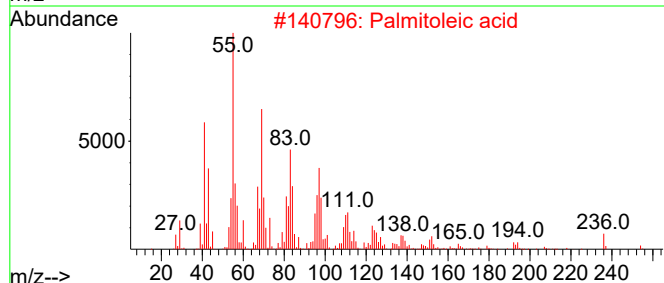
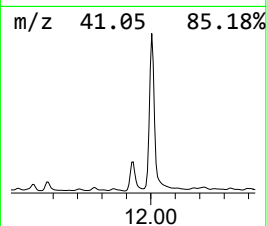
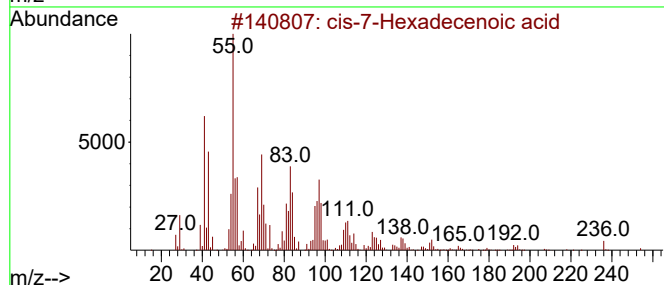
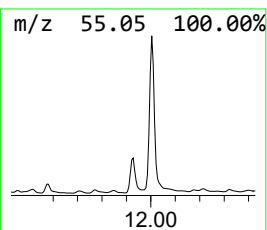
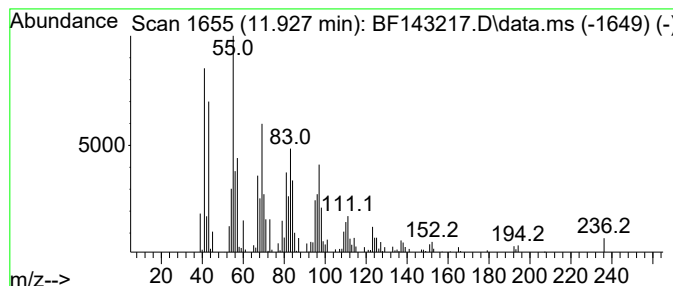
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 cis-7-Hexadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	3.31 ng	186933	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	95
2			Palmitoleic acid	254	C16H30O2	000373-49-9	93
3			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	93
4			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	87
5			Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	62



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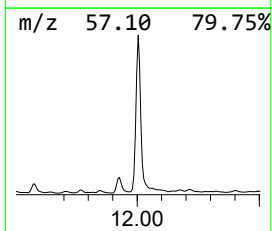
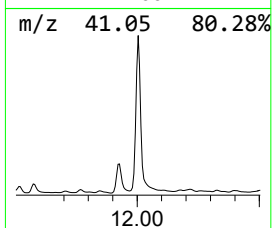
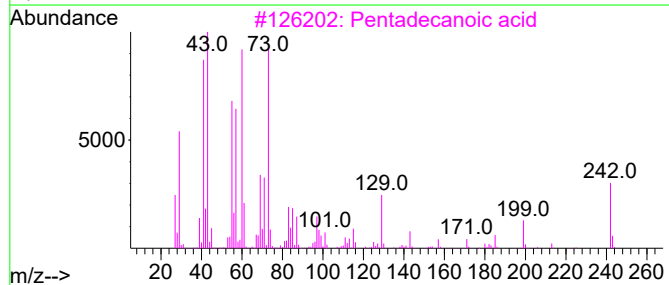
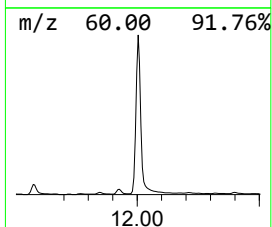
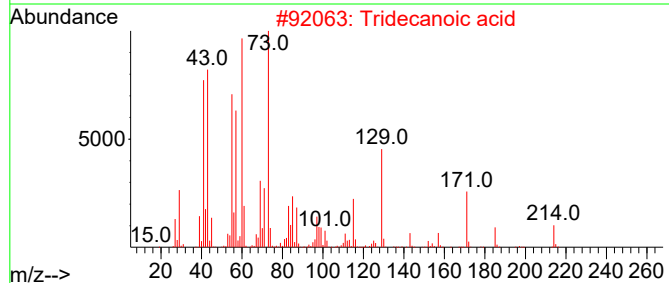
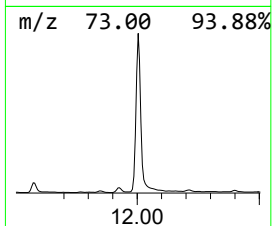
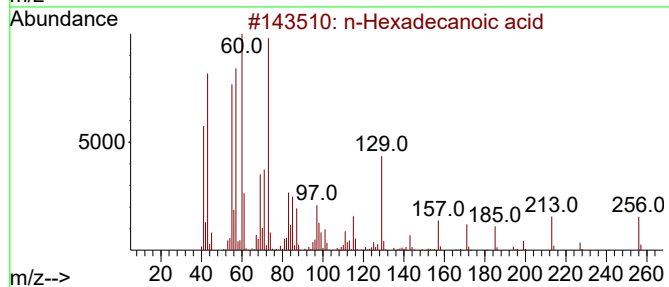
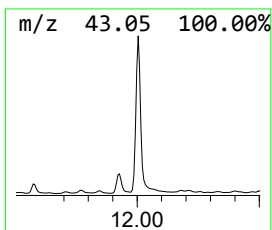
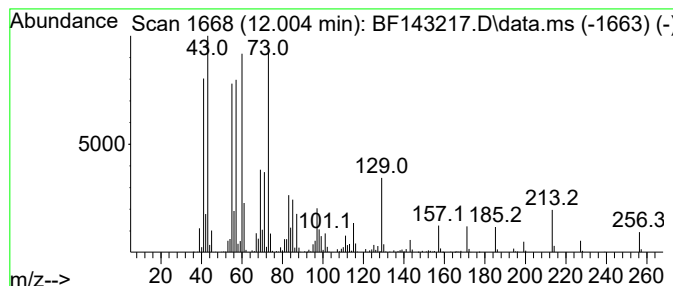
Instrument :
BNA_F
ClientSampleId :
WC-2

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 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.004	16.75 ng	945187	Phenanthrene-d10	11.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072325\
Data File : BF143217.D
Acq On : 23 Jul 2025 17:57
Operator : RC/JU
Sample : Q2649-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

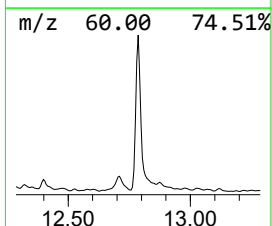
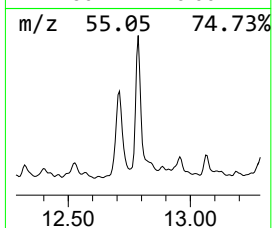
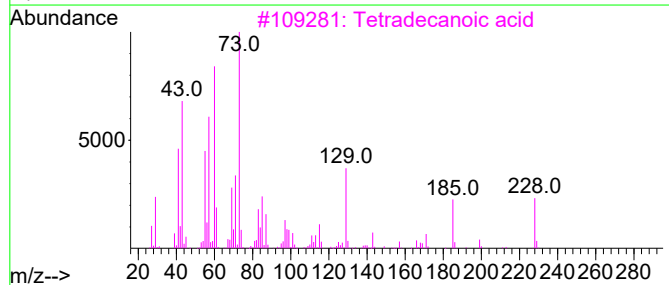
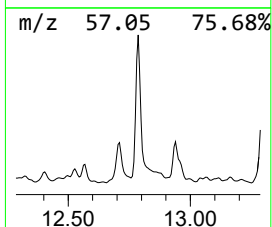
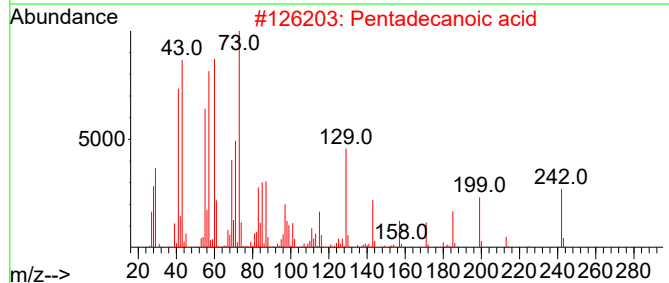
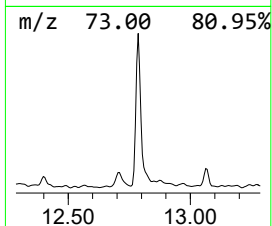
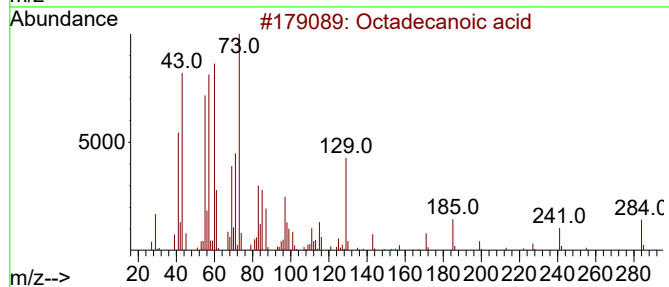
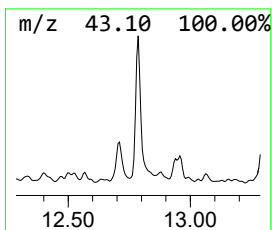
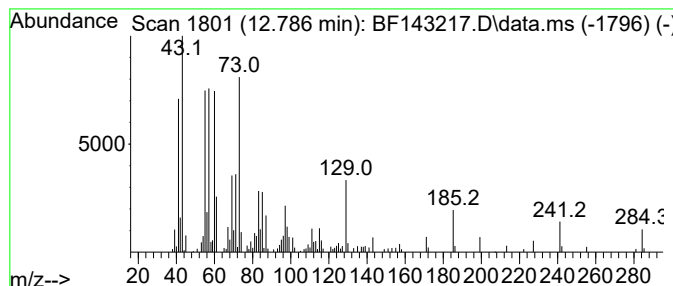
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	3.11 ng	175681	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	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072325\
Data File : BF143217.D
Acq On : 23 Jul 2025 17:57
Operator : RC/JU
Sample : Q2649-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

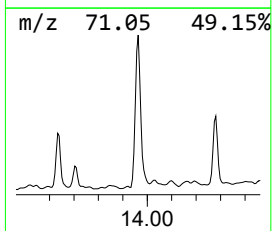
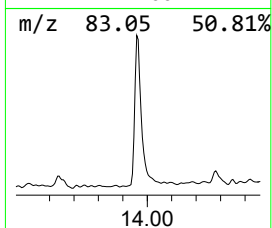
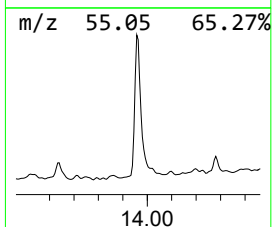
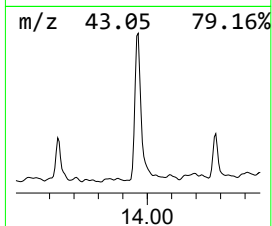
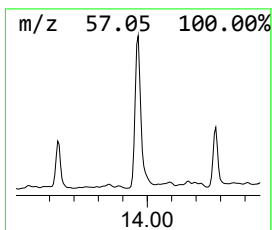
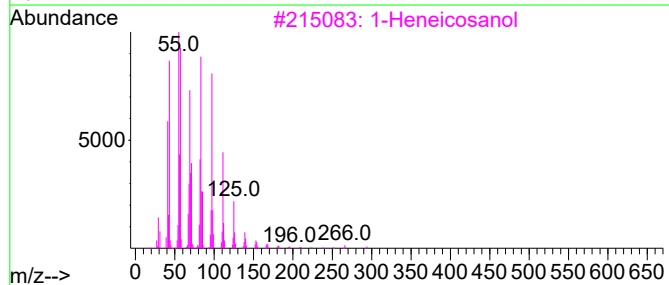
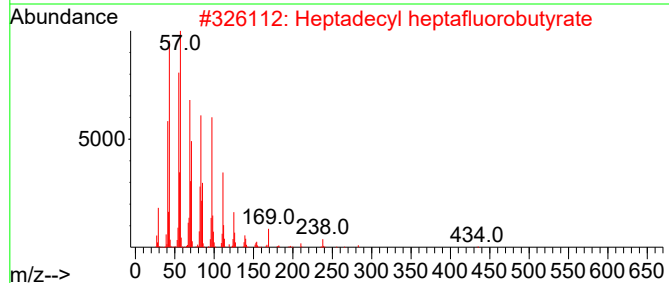
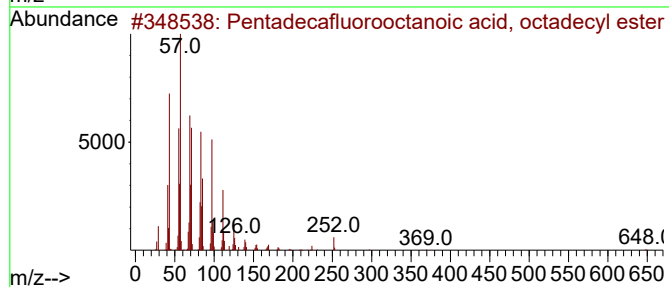
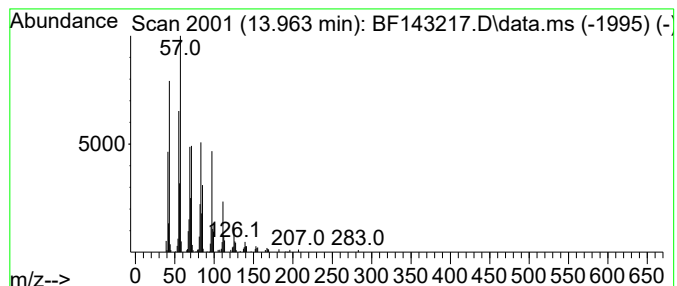
Instrument :
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ClientSampleId :
WC-2

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 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.963	6.92 ng	248924	Chrysene-d12	14.121	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072325\
Data File : BF143217.D
Acq On : 23 Jul 2025 17:57
Operator : RC/JU
Sample : Q2649-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

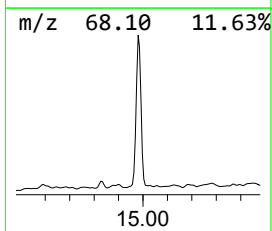
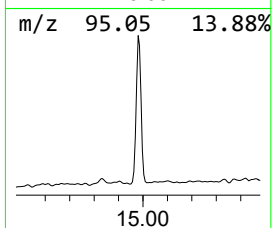
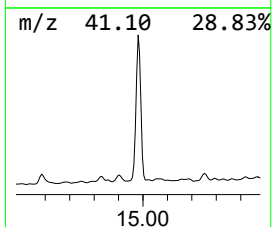
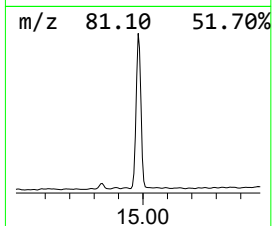
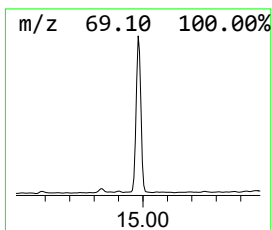
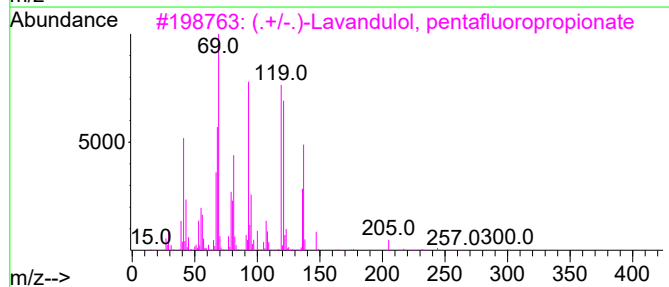
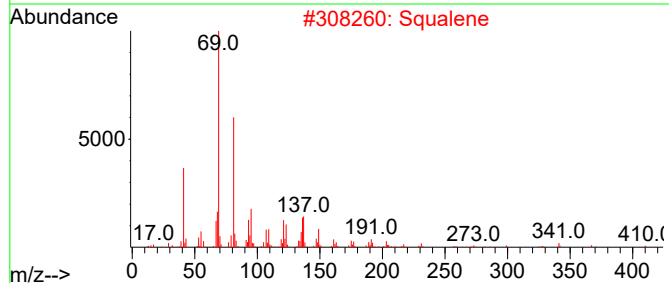
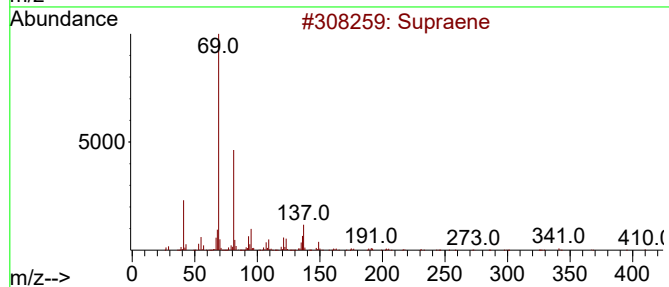
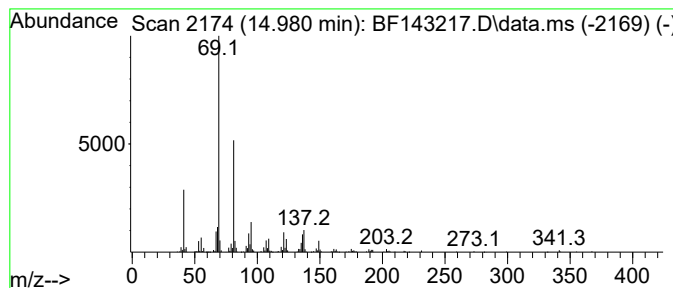
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	10.49 ng	384157	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
4			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072325\
Data File : BF143217.D
Acq On : 23 Jul 2025 17:57
Operator : RC/JU
Sample : Q2649-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

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...	2.316	33.9	ng	1312770	1	6.963	775082	20.0
2-Pentanone, 4-...	5.198	10.6	ng	411515	1	6.963	775082	20.0
Benzophenone	10.704	11.7	ng	662032	3	9.998	1132960	20.0
Tetradecanoic acid	11.139	2.5	ng	138709	4	11.480	1128580	20.0
cis-7-Hexadecen...	11.927	3.3	ng	186933	4	11.480	1128580	20.0
n-Hexadecanoic ...	12.004	16.8	ng	945187	4	11.480	1128580	20.0
Octadecanoic acid	12.786	3.1	ng	175681	4	11.480	1128580	20.0
Pentadecafluoro...	13.963	6.9	ng	248924	5	14.121	719076	20.0
Supraene	14.980	10.5	ng	384157	6	15.621	732229	20.0