

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
 Data File : BF142650.D
 Acq On : 06 Jun 2025 17:01
 Operator : RC/JU
 Sample : Q2176-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-31

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-BF052025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142650.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	487	496	511	rBV	180573	280061	9.51%	1.315%
2	5.510	558	564	570	rBV	1712436	2358708	80.13%	11.076%
3	6.516	729	735	760	rVB	1713445	2424824	82.38%	11.386%
4	6.892	794	799	804	rBV	594500	724569	24.62%	3.402%
5	7.457	888	895	900	rBV	1122470	1554116	52.80%	7.297%
6	8.175	1012	1017	1032	rBV	720815	958779	32.57%	4.502%
7	9.251	1194	1200	1205	rBV	2330068	2943523	100.00%	13.822%
8	9.933	1311	1316	1321	rBV	883126	1082241	36.77%	5.082%
9	10.645	1432	1437	1443	rBV	543722	685334	23.28%	3.218%
10	10.722	1445	1450	1465	rVB	1446521	1908720	64.84%	8.963%
11	10.957	1481	1490	1494	rBV	88685	110778	3.76%	0.520%
12	11.422	1564	1569	1578	rBV2	790287	1130929	38.42%	5.310%
13	11.645	1602	1607	1615	rBV3	35983	65244	2.22%	0.306%
14	11.945	1650	1658	1665	rBV2	175566	291561	9.91%	1.369%
15	12.039	1670	1674	1682	rVB3	24704	51819	1.76%	0.243%
16	12.198	1696	1701	1708	rBV3	46486	68084	2.31%	0.320%
17	12.463	1738	1746	1752	rBV3	78169	150361	5.11%	0.706%
18	12.639	1771	1776	1784	rBV	88667	126501	4.30%	0.594%
19	12.727	1787	1791	1799	rVV	24716	41980	1.43%	0.197%
20	12.863	1808	1814	1818	rBV2	67367	111025	3.77%	0.521%
21	13.010	1833	1839	1847	rBV	1725667	2241732	76.16%	10.526%
22	13.210	1863	1873	1880	rBV5	34864	101915	3.46%	0.479%
23	13.310	1888	1890	1895	rVB2	25283	31998	1.09%	0.150%
24	13.898	1986	1990	2005	rVB2	113755	201696	6.85%	0.947%
25	14.063	2013	2018	2029	rVB	481166	721507	24.51%	3.388%
26	14.539	2095	2099	2113	rVB3	37397	89793	3.05%	0.422%
27	14.921	2160	2164	2168	rVB	24925	32810	1.11%	0.154%
28	15.121	2193	2198	2206	rBV	25893	60679	2.06%	0.285%
29	15.563	2266	2273	2286	rVB	441195	745320	25.32%	3.500%

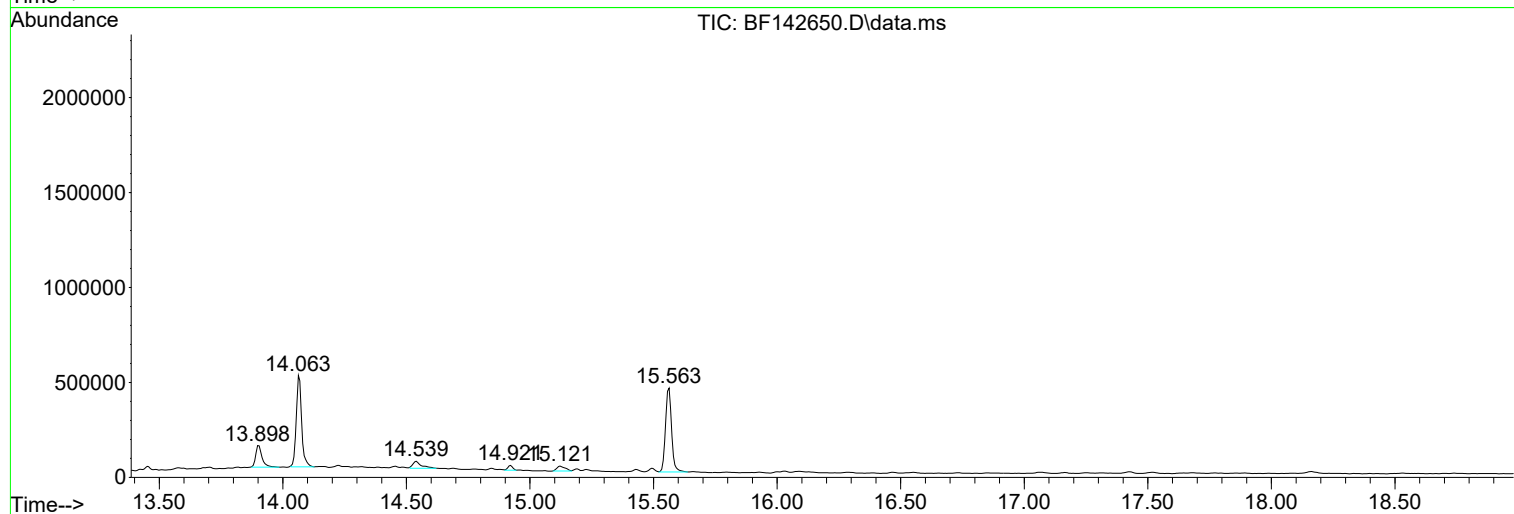
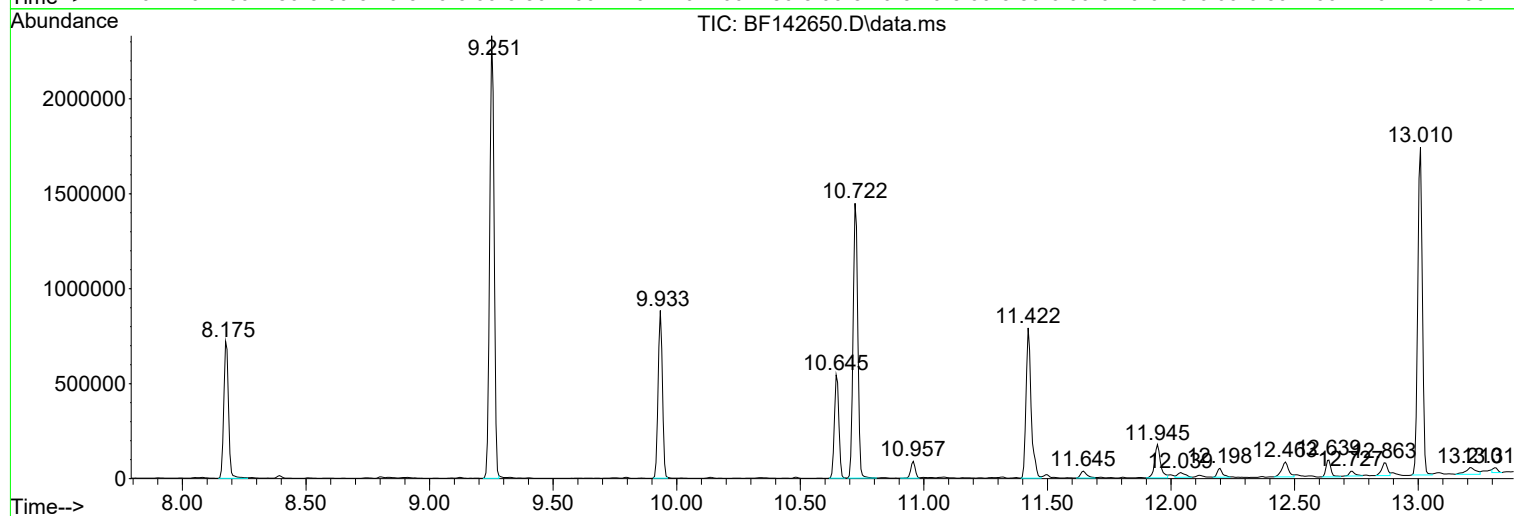
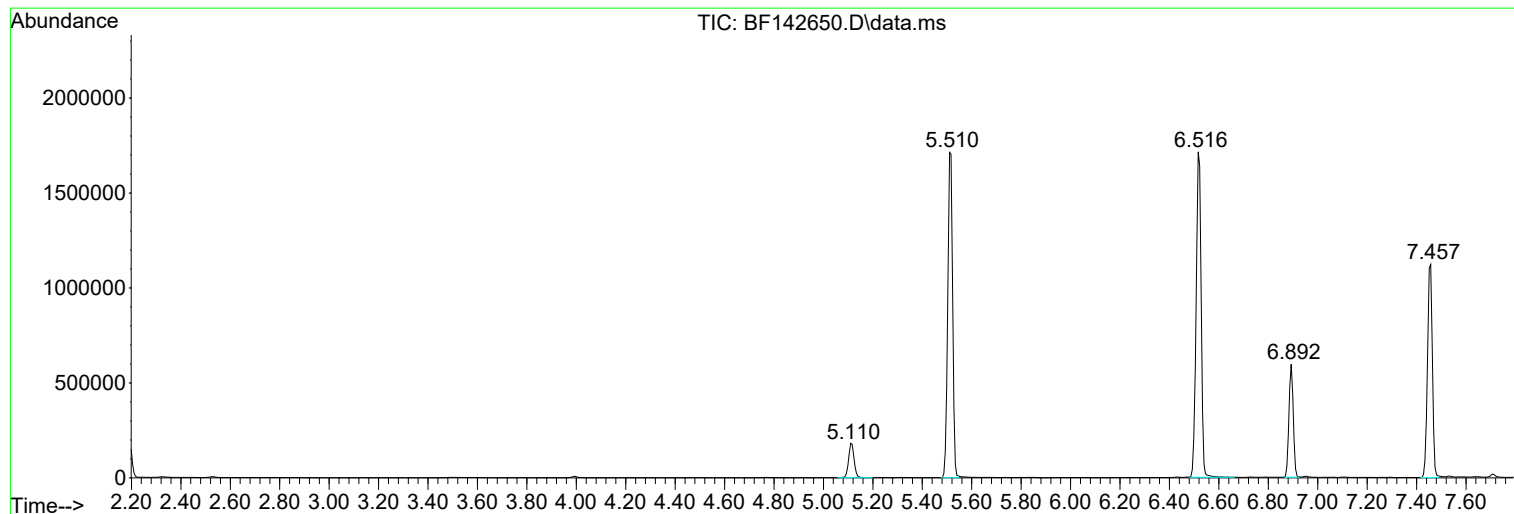
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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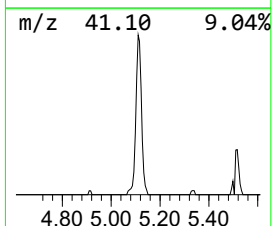
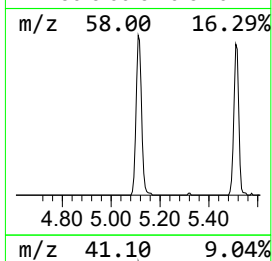
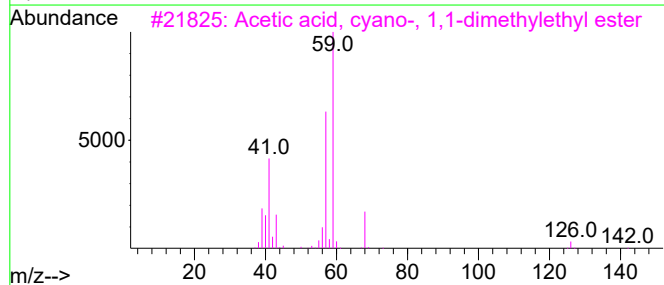
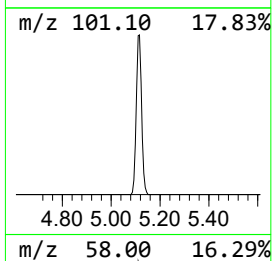
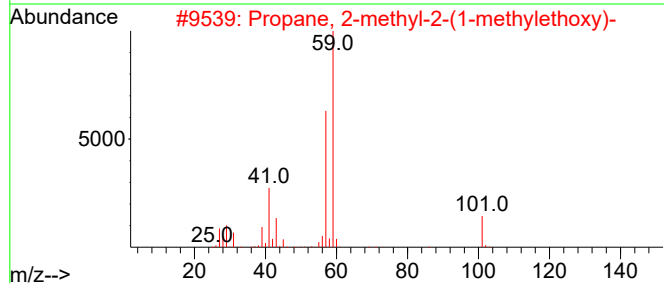
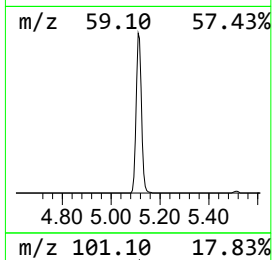
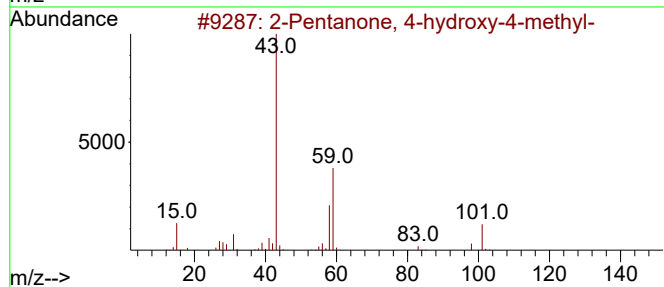
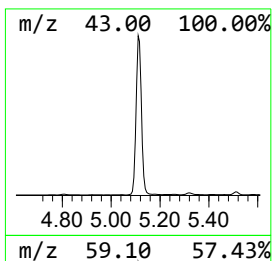
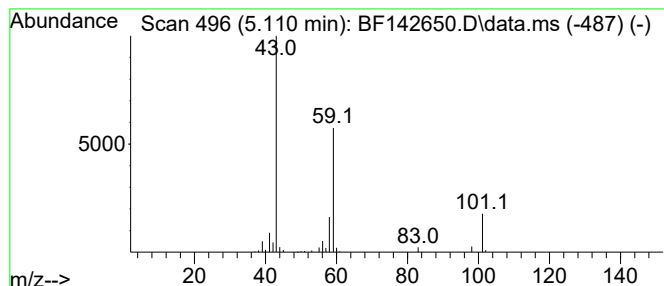
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	7.73 ng	280061	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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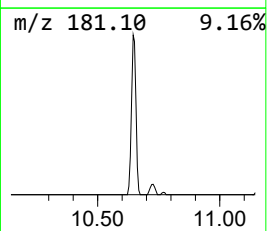
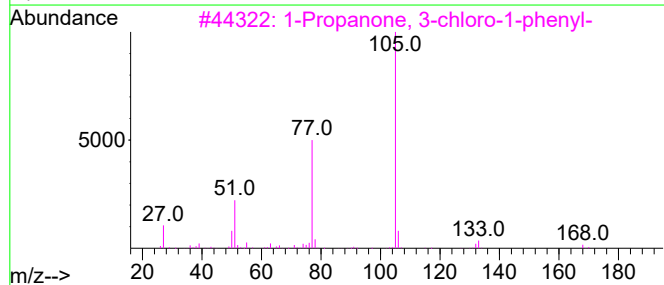
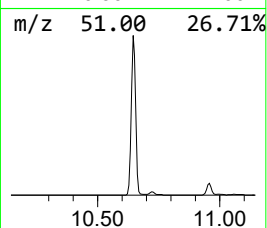
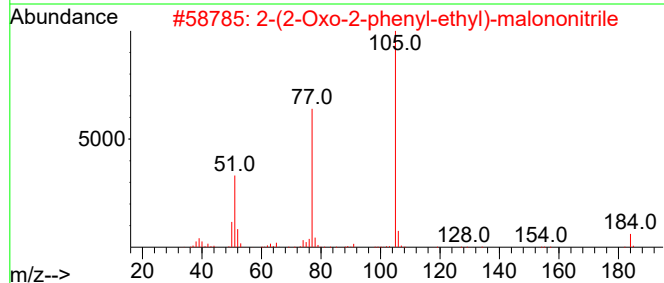
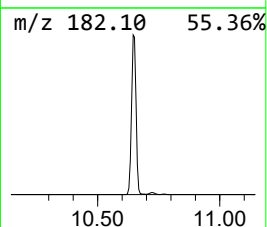
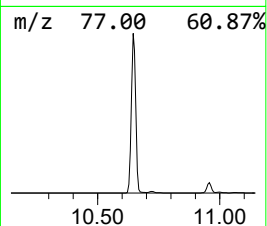
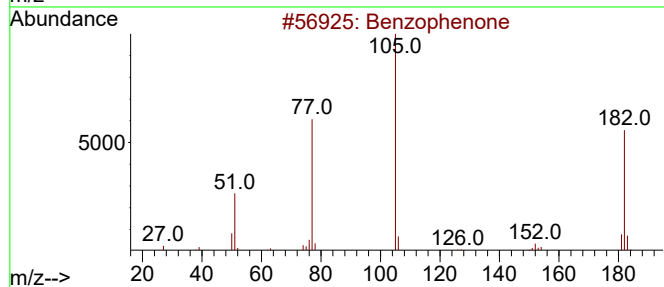
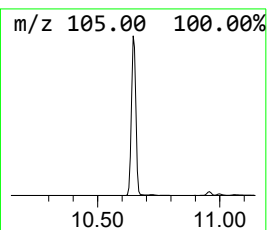
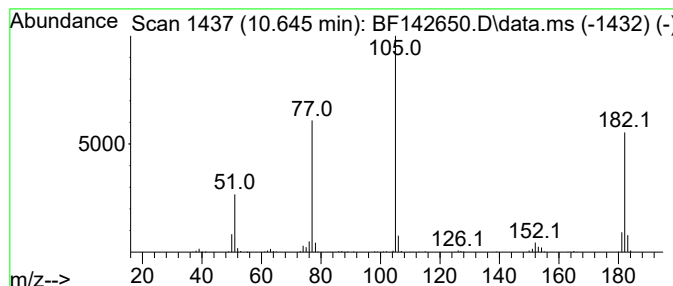
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	12.67 ng	685334	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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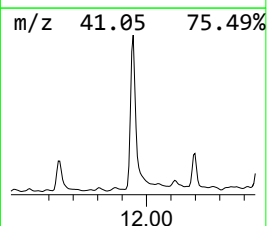
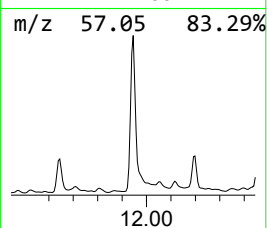
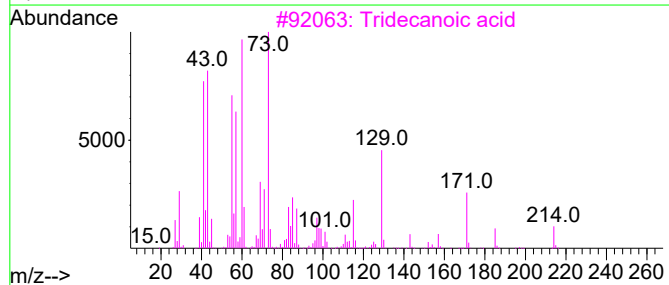
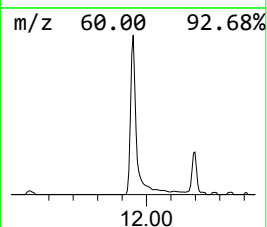
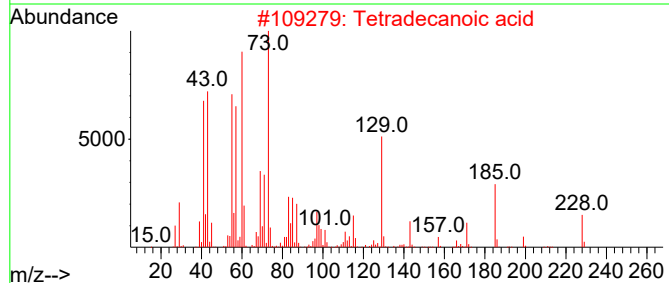
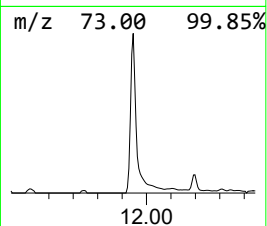
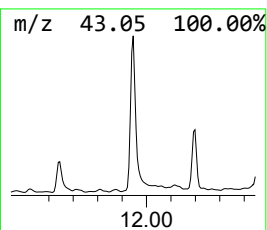
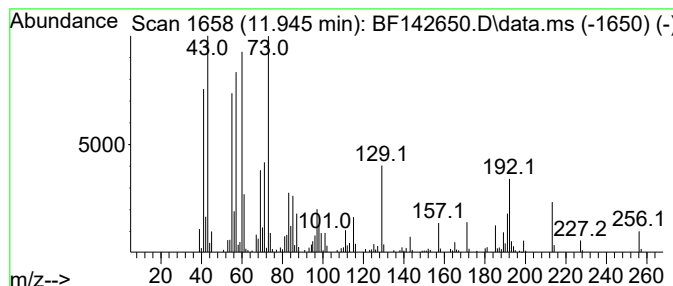
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	5.16 ng	291561	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



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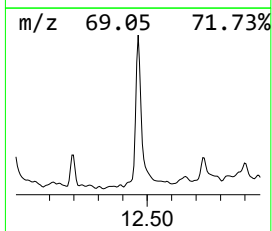
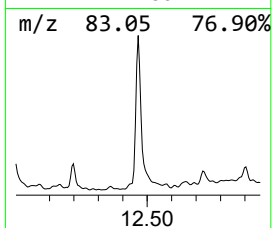
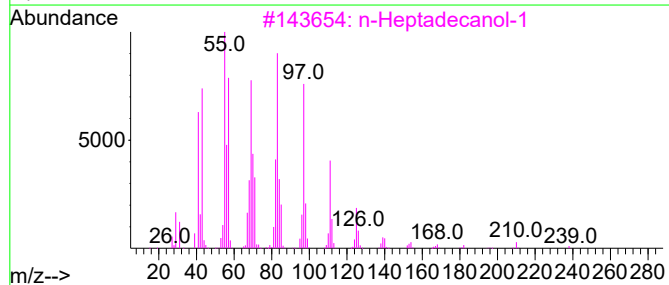
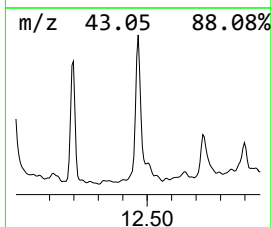
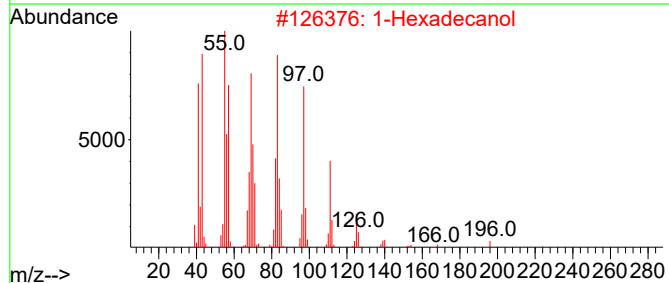
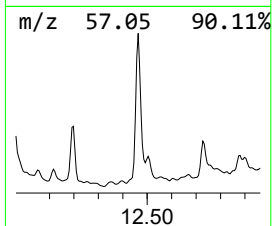
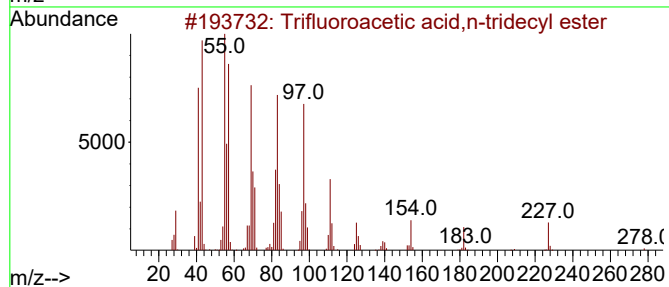
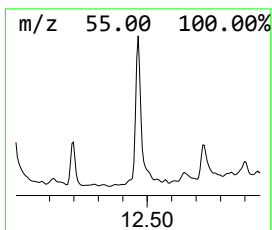
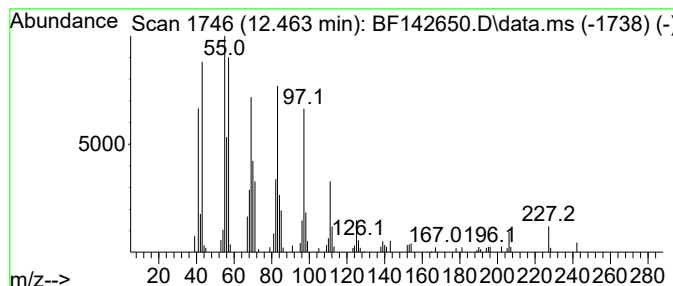
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Peak Number 4 Trifluoroacetic acid,n-trid... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	2.66 ng	150361	Phenanthrene-d10	11.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	94
2		1-Hexadecanol	242	C16H34O	036653-82-4	93
3		n-Heptadecanol-1	256	C17H36O	001454-85-9	93
4		1-Octadecanol	270	C18H38O	000112-92-5	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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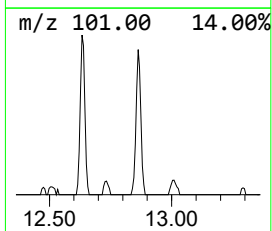
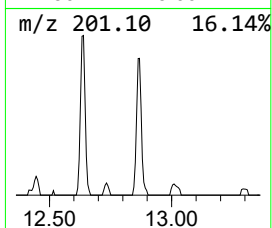
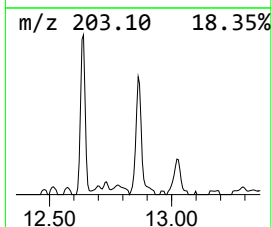
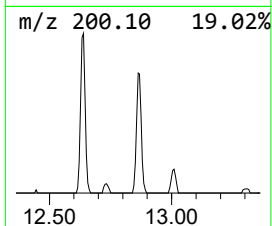
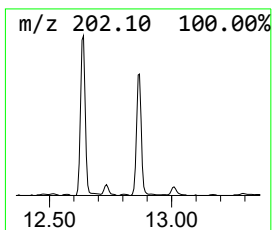
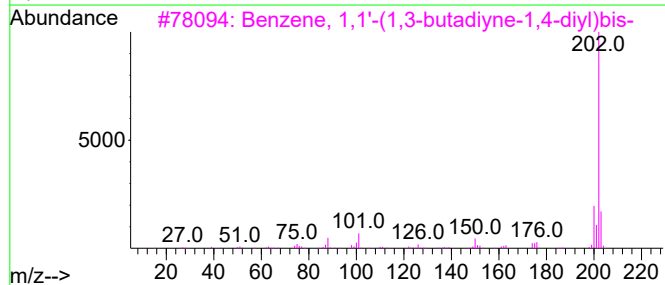
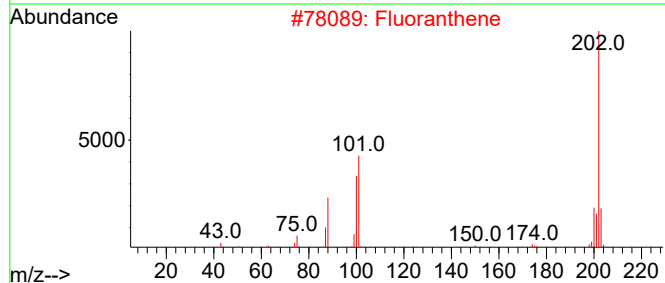
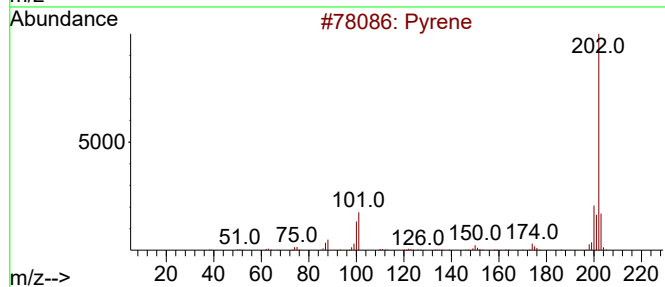
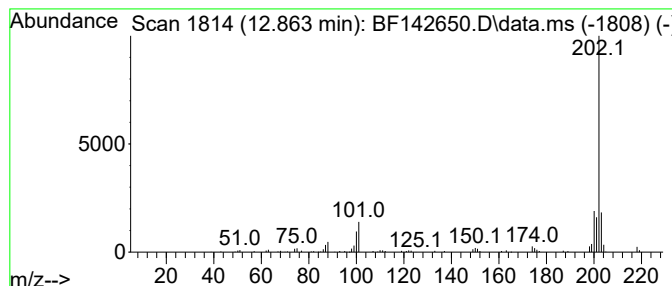
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Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.863	3.08 ng	111025	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	96
2	Fluoranthene	202	C16H10	000206-44-0	93
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4	Pyrimidine, 2-phenyl-4-hydroxy-5...	202	C11H10N2O2	085386-21-6	9
5	5-Ethyl-4,7-dihydro-2-methyl-7-o...	202	C10H10N4O	903195-75-5	9



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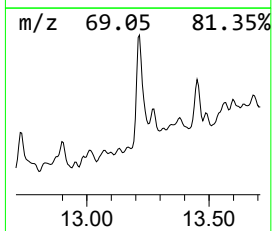
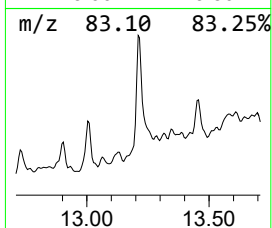
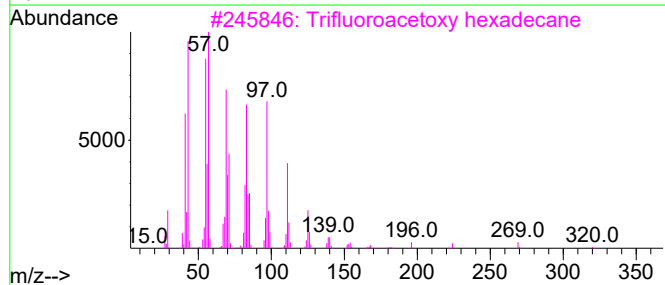
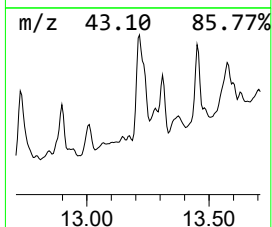
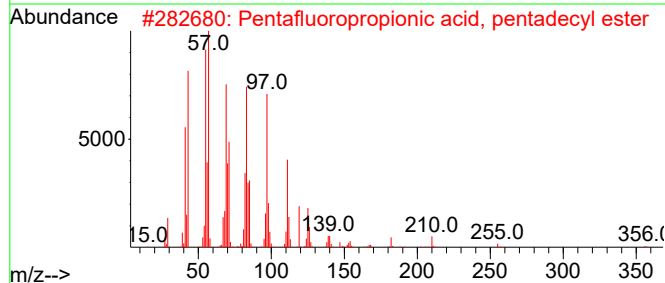
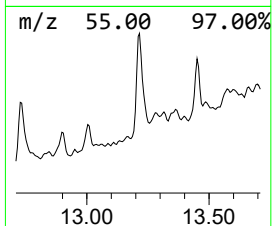
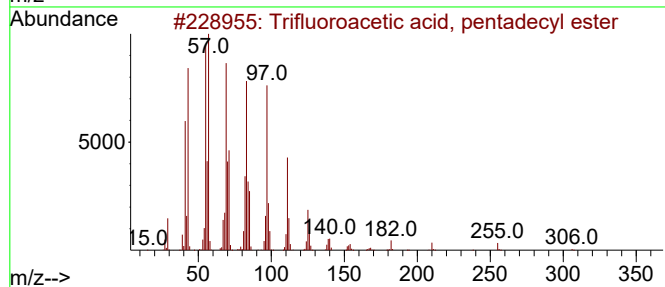
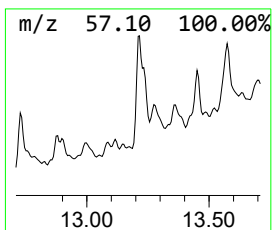
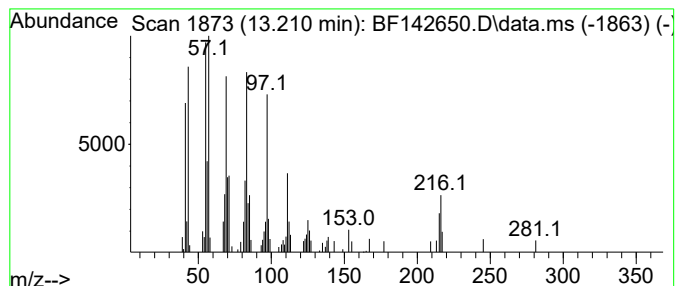
Instrument :
BNA_F
ClientSampleId :
TP-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.210	2.83 ng	101915	Chrysene-d12		14.063	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	93
2	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	93
3	Trifluoroacetoxo hexadecane		338	C18H33F3O2	006222-03-3	93
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	90
5	Behenic alcohol		326	C22H46O	000661-19-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142650.D
Acq On : 06 Jun 2025 17:01
Operator : RC/JU
Sample : Q2176-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

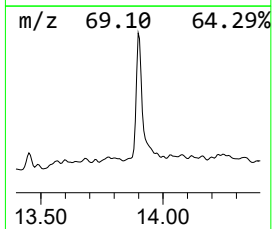
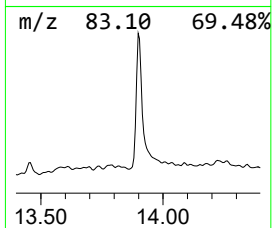
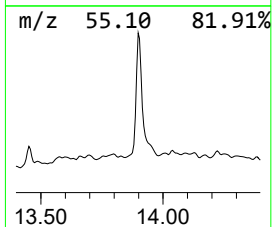
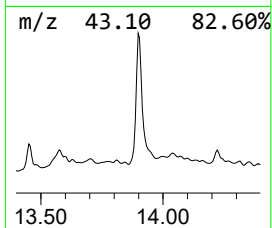
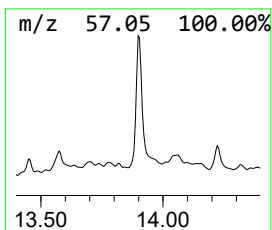
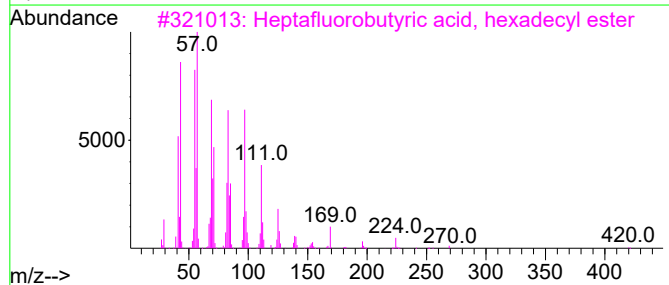
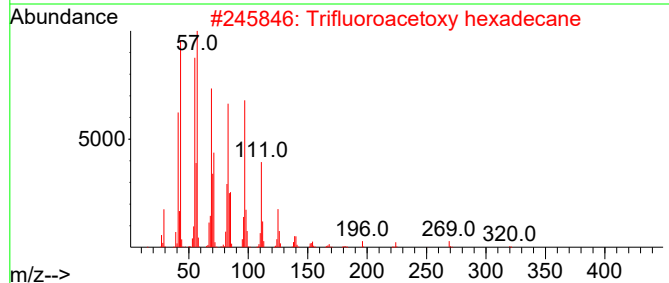
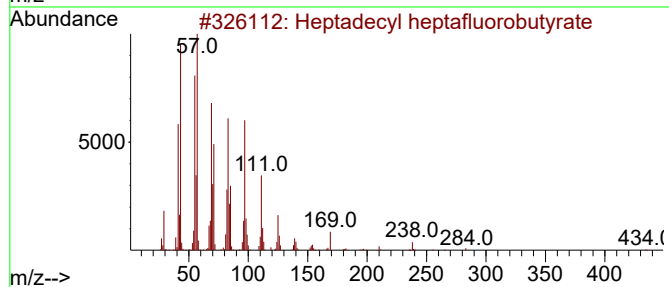
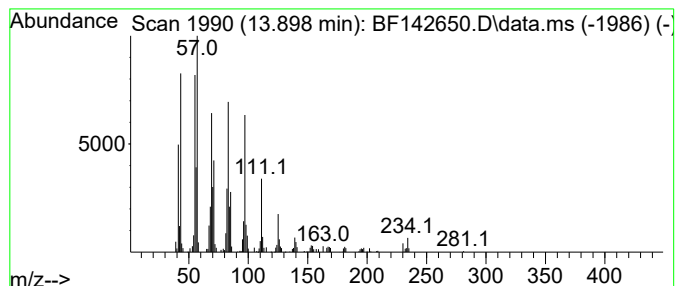
Instrument :
BNA_F
ClientSampleId :
TP-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	5.59 ng	201696	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142650.D
Acq On : 06 Jun 2025 17:01
Operator : RC/JU
Sample : Q2176-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-31

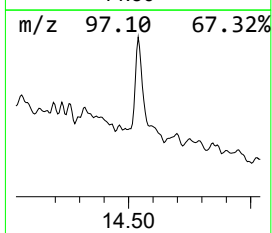
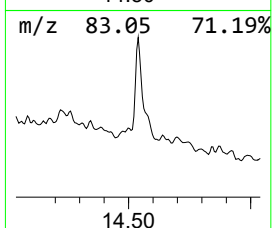
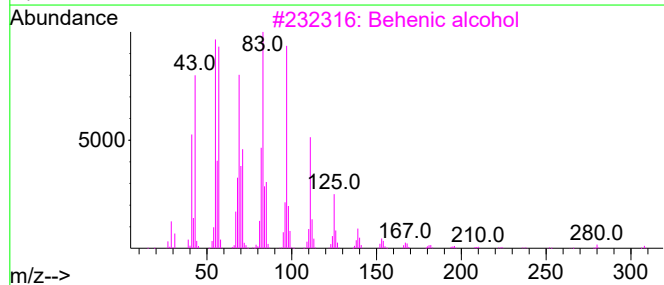
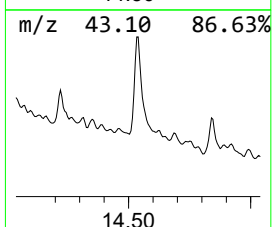
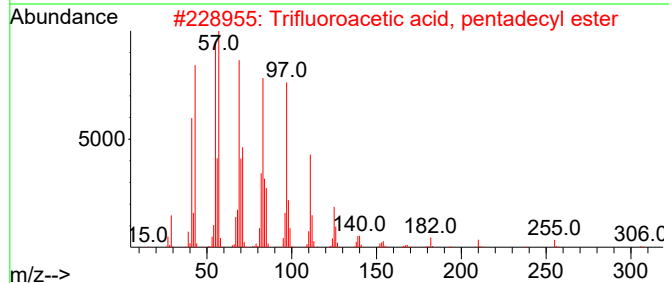
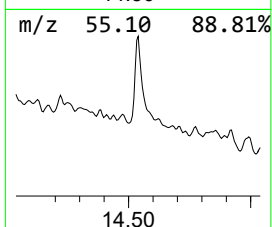
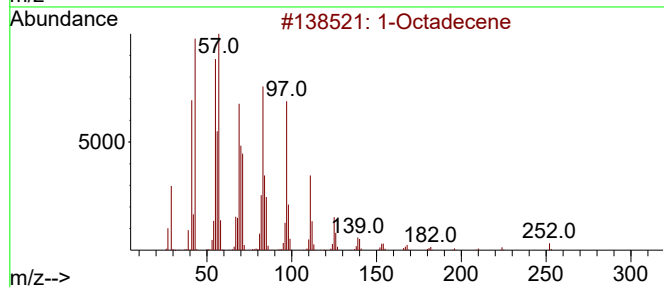
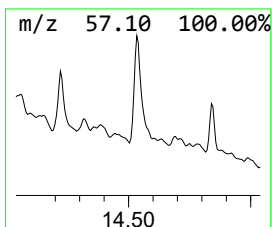
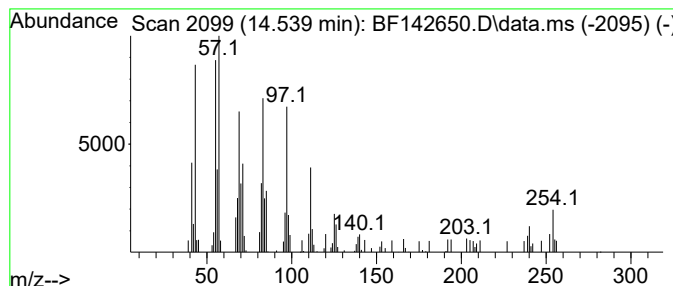
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	2.49 ng	89793	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene			252	C18H36	000112-88-9	98
2	Trifluoroacetic acid, pentadecyl...			324	C17H31F3O2	959010-23-2	93
3	Behenic alcohol			326	C22H46O	000661-19-8	93
4	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	93
5	Heptafluorobutyric acid, hexadec...			438	C20H33F7O2	006385-15-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142650.D
Acq On : 06 Jun 2025 17:01
Operator : RC/JU
Sample : Q2176-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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
2-Pentanone, 4-...	5.110	7.7	ng	280061	1	6.892	724569	20.0
Benzophenone	10.645	12.7	ng	685334	3	9.933	1082240	20.0
n-Hexadecanoic ...	11.945	5.2	ng	291561	4	11.422	1130930	20.0
Trifluoroacetic...	12.463	2.7	ng	150361	4	11.422	1130930	20.0
Benzene, 1,1'-(...	12.863	3.1	ng	111025	5	14.063	721507	20.0
Trifluoroacetic...	13.210	2.8	ng	101915	5	14.063	721507	20.0
Heptadecyl hept...	13.898	5.6	ng	201696	5	14.063	721507	20.0
1-Octadecene	14.539	2.5	ng	89793	5	14.063	721507	20.0