

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
 Data File : BF141765.D
 Acq On : 25 Feb 2025 15:35
 Operator : RC/JU
 Sample : Q1421-09
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-CLAY-CF02-01

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	488	492	508	rVB	39125	71829	3.43%	0.557%
2	5.404	558	563	586	rBV	1169611	1714865	81.81%	13.302%
3	6.422	731	736	766	rBV	1197309	1736778	82.86%	13.472%
4	6.781	792	797	805	rBV	320221	409394	19.53%	3.176%
5	7.345	887	893	921	rBV	794136	1135733	54.18%	8.810%
6	7.634	935	942	960	rBV3	11180	35256	1.68%	0.273%
7	8.063	1010	1015	1040	rBV	379410	549249	26.20%	4.261%
8	9.134	1192	1197	1209	rBV	1598723	2096123	100.00%	16.260%
9	9.816	1307	1313	1330	rBV	425209	601858	28.71%	4.669%
10	10.528	1429	1434	1442	rBV	100126	135182	6.45%	1.049%
11	10.604	1442	1447	1462	rVV	685493	970814	46.31%	7.531%
12	10.839	1483	1487	1496	rVB	14844	21217	1.01%	0.165%
13	11.298	1560	1565	1581	rVB	376460	556798	26.56%	4.319%
14	11.833	1651	1656	1668	rBV3	26617	71748	3.42%	0.557%
15	12.880	1829	1834	1852	rBV	1315931	1720467	82.08%	13.346%
16	13.786	1983	1988	2005	rBV3	29164	113601	5.42%	0.881%
17	13.939	2009	2014	2025	rVB	281564	404524	19.30%	3.138%
18	14.692	2137	2142	2149	rBV2	24270	44819	2.14%	0.348%
19	14.774	2151	2156	2161	rVB	39617	57775	2.76%	0.448%
20	15.386	2254	2260	2271	rBV	253185	443457	21.16%	3.440%

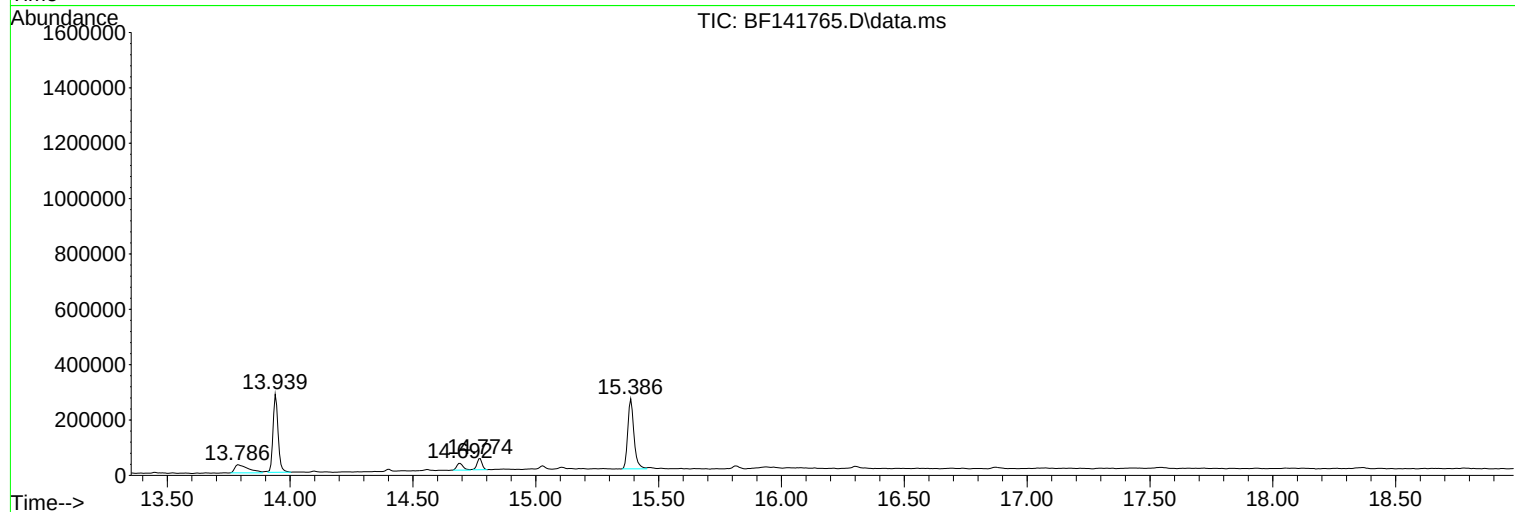
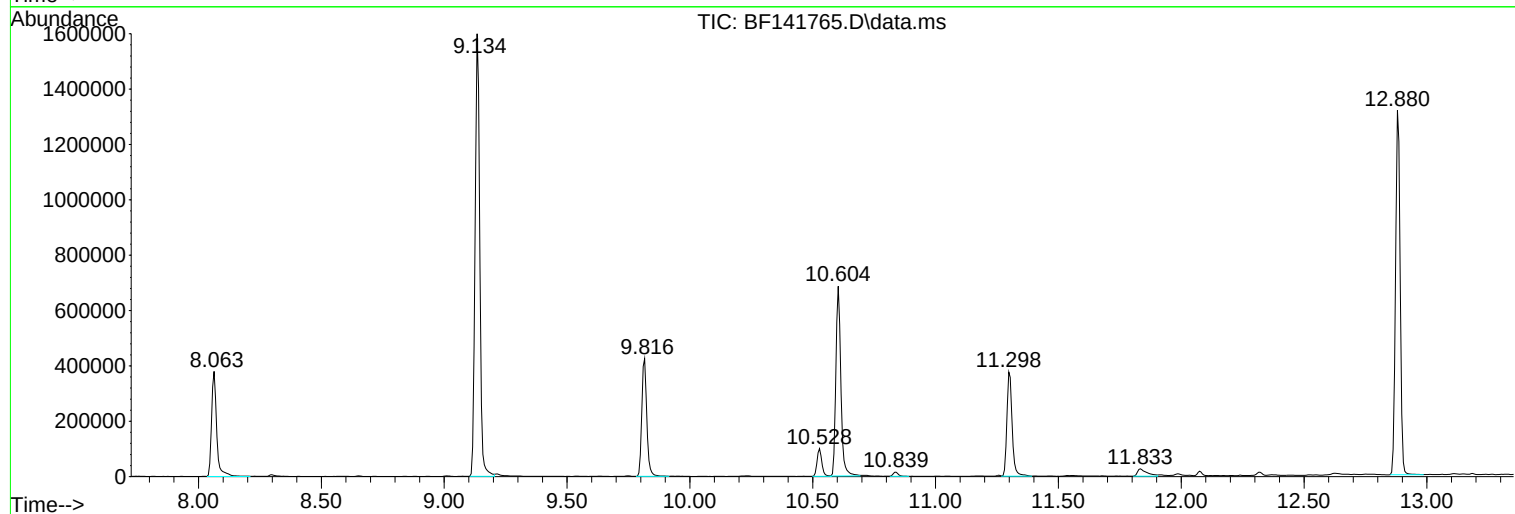
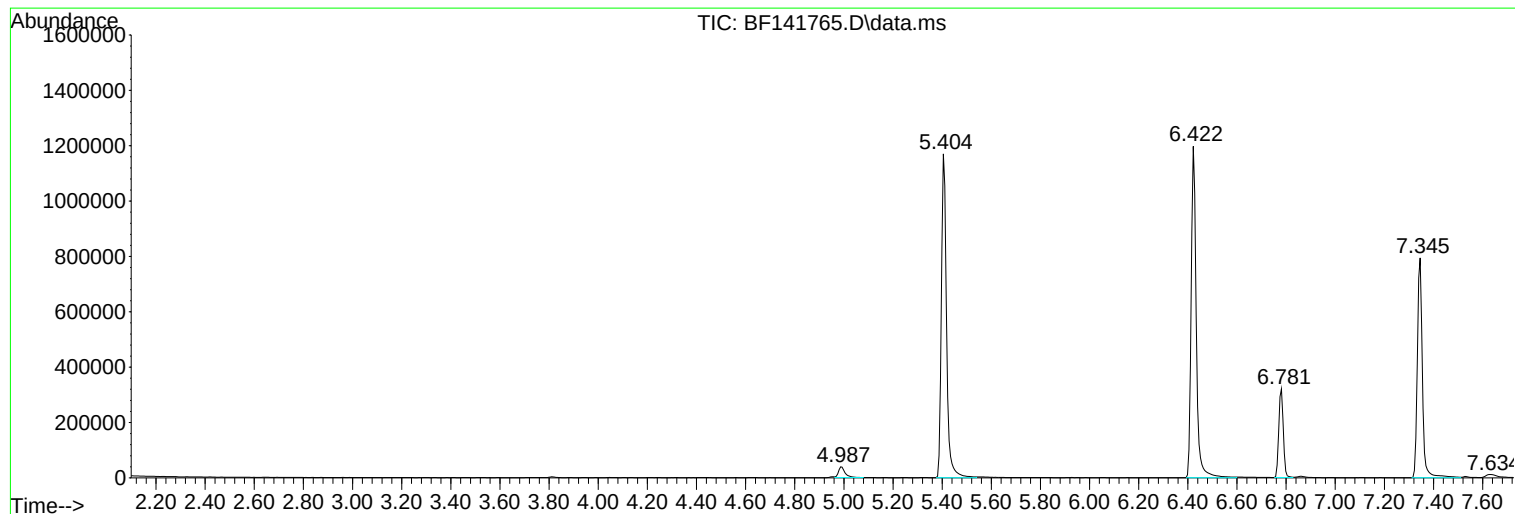
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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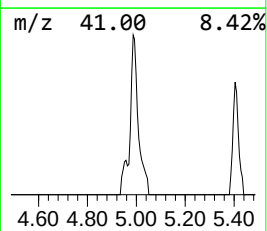
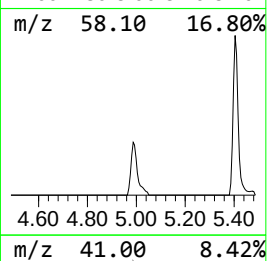
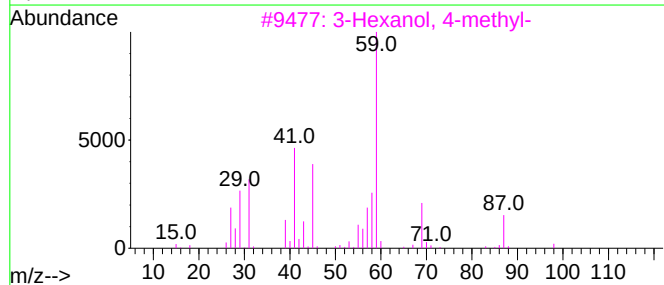
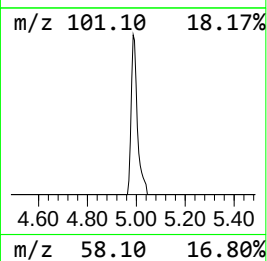
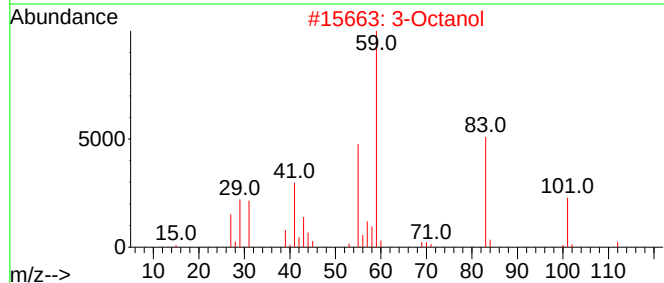
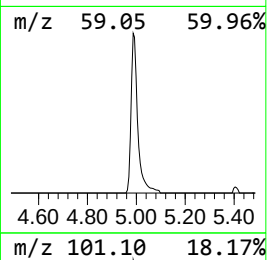
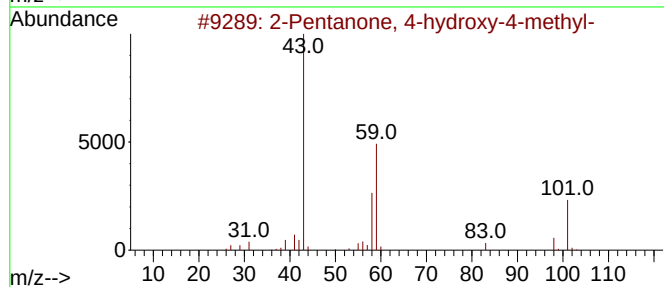
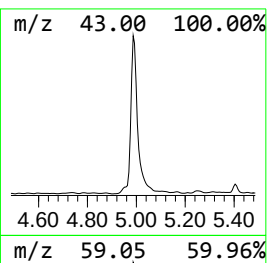
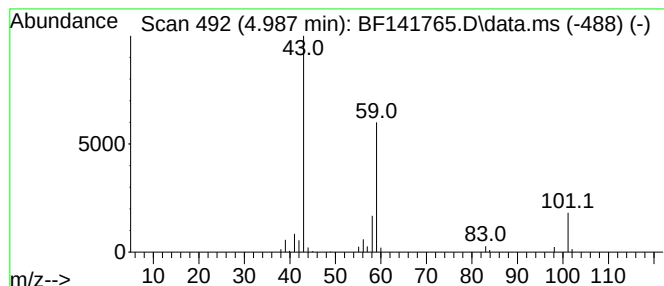
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	3.51 ng	71829	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	3-Octanol	130	C8H18O	000589-98-0	36	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23	



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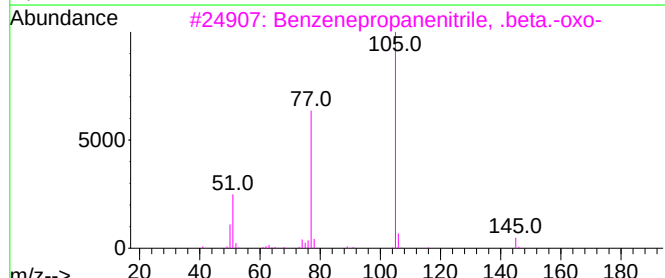
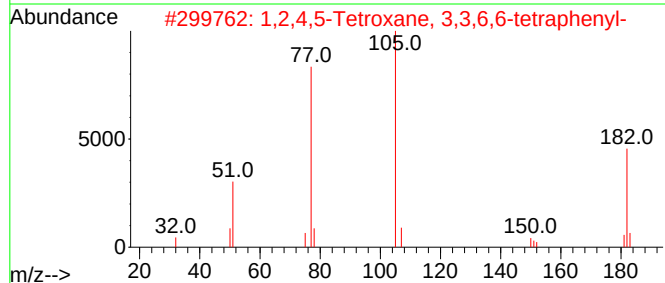
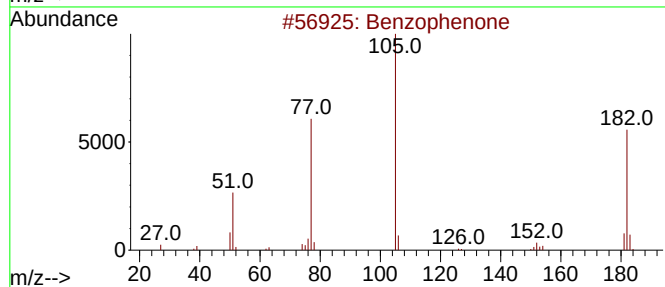
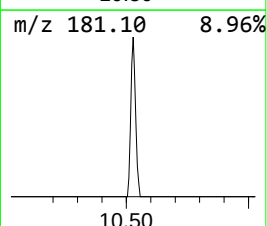
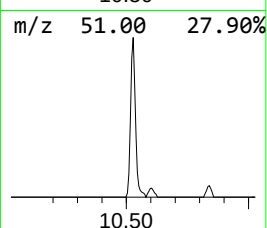
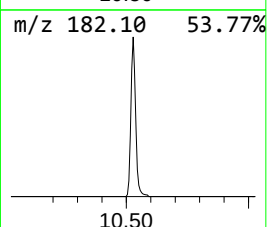
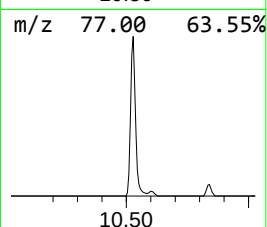
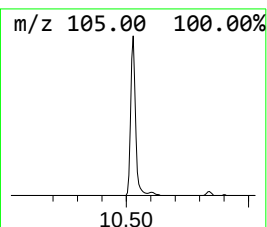
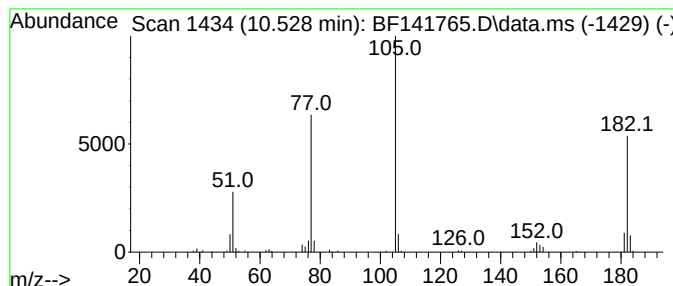
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.528	4.49 ng	135182	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	49
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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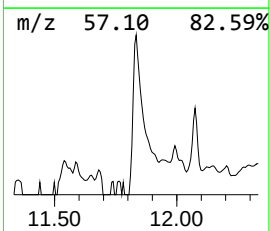
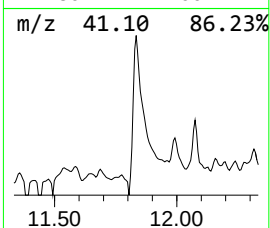
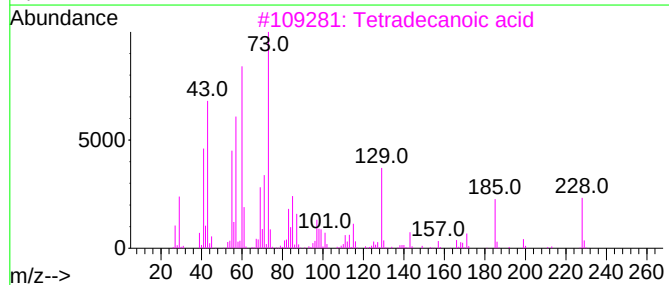
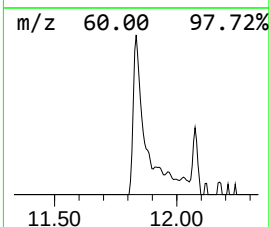
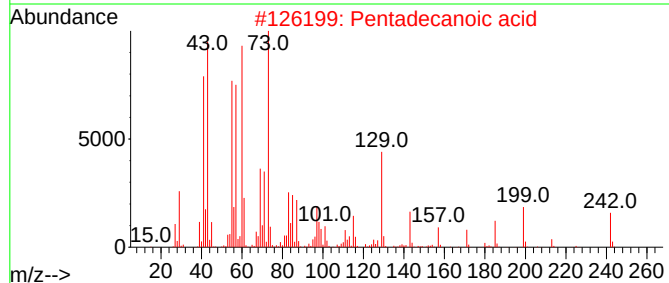
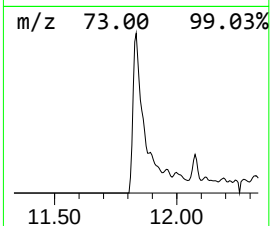
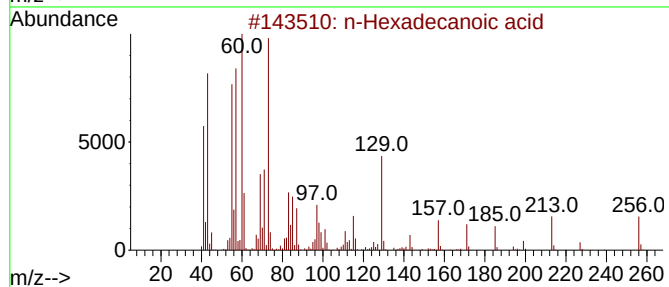
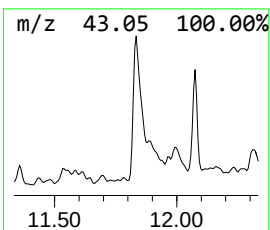
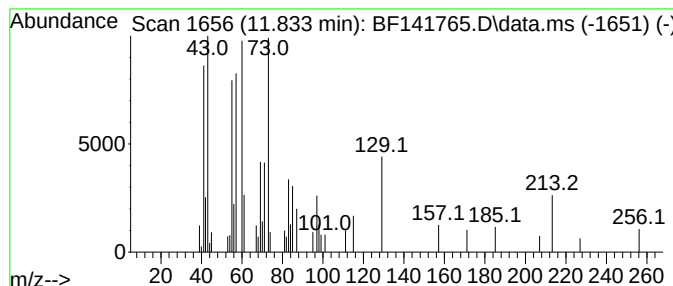
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.58 ng	71748	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Undecanoic acid	186	C11H22O2	000112-37-8	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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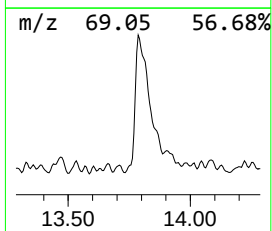
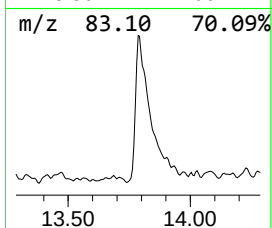
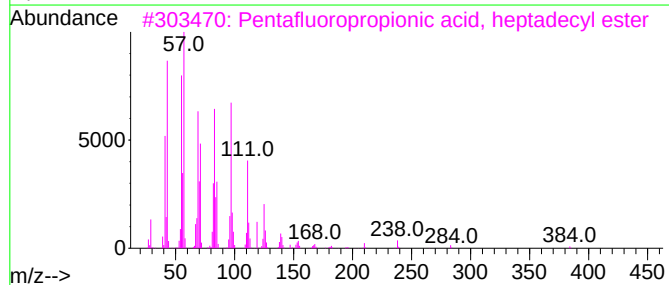
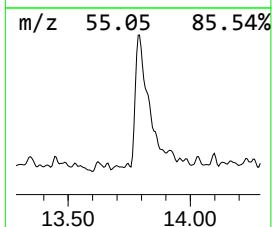
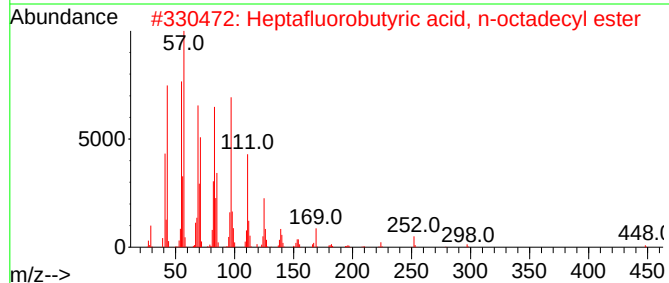
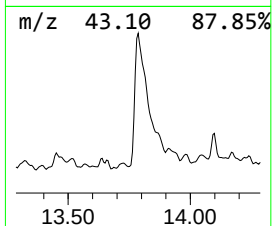
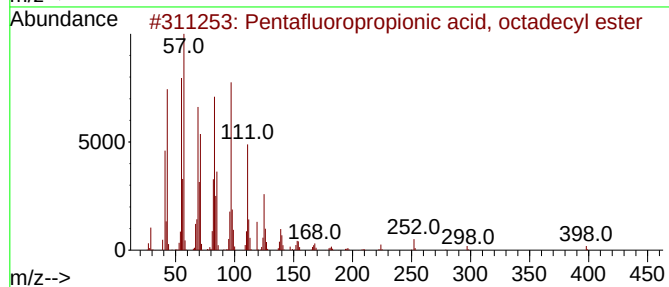
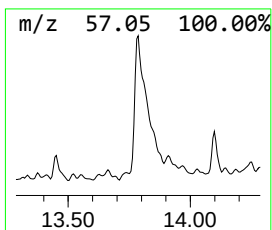
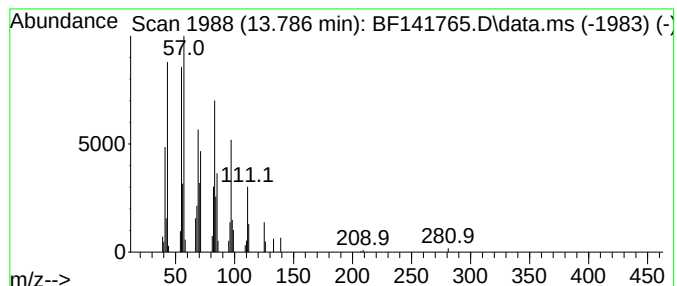
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	5.62 ng	113601	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91



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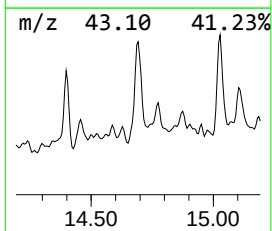
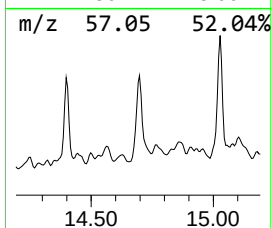
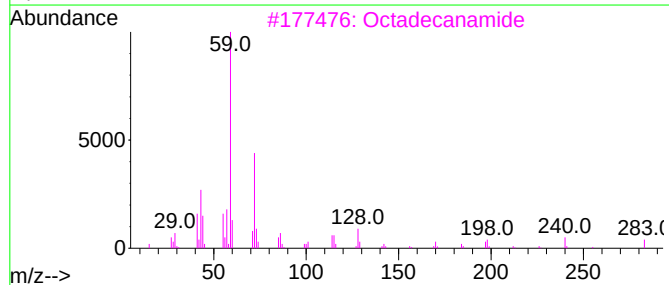
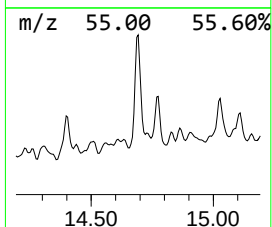
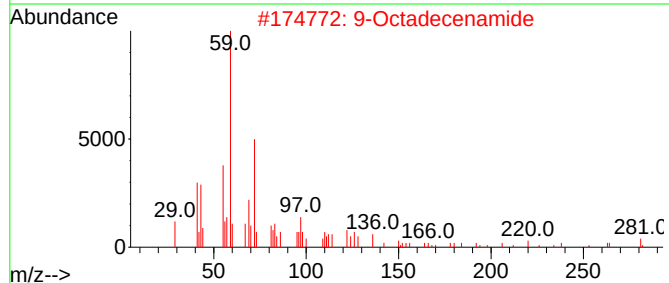
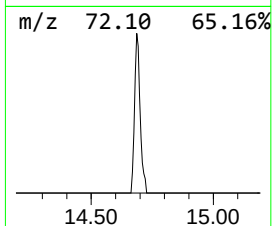
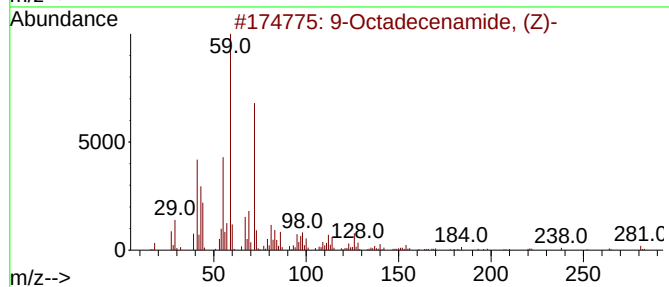
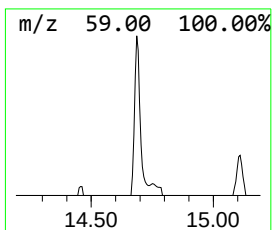
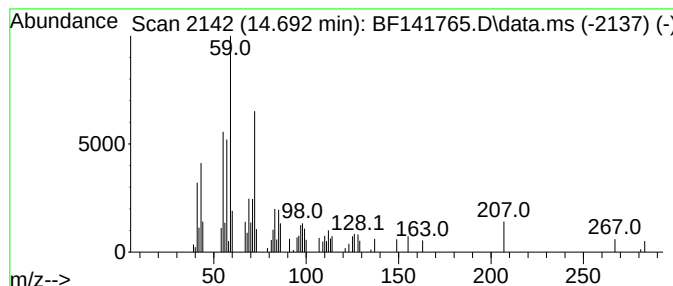
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	2.02 ng	44819	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			9-Octadecenamide	281	C18H35NO	003322-62-1	53
3			Octadecanamide	283	C18H37NO	000124-26-5	52
4			d-Glucosamine	179	C6H13NO5	000090-77-7	50
5			4-Pentenoic acid, methyl ester	114	C6H10O2	000818-57-5	49



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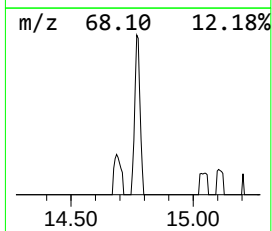
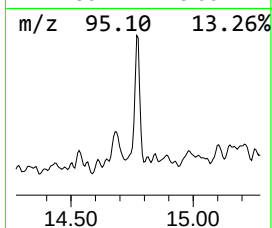
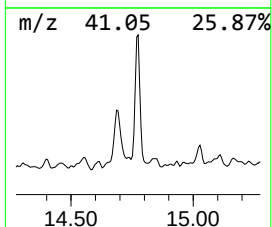
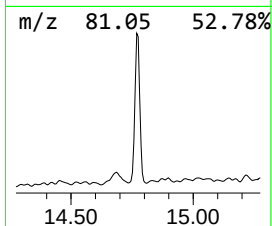
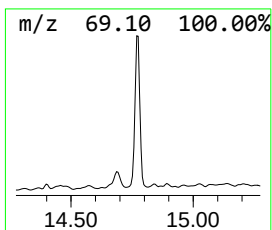
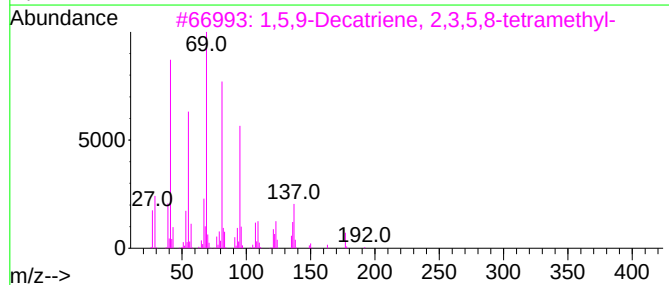
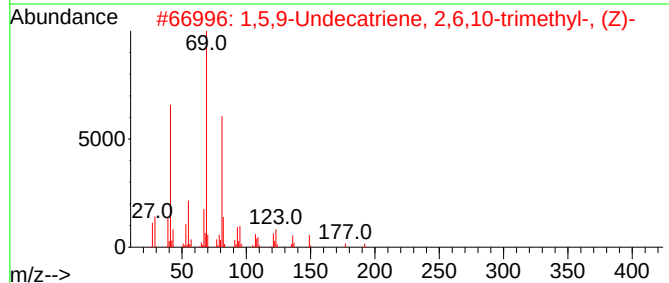
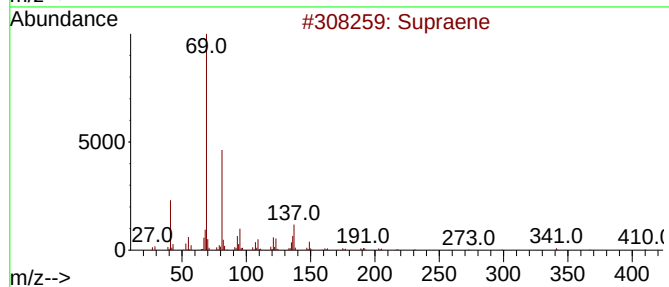
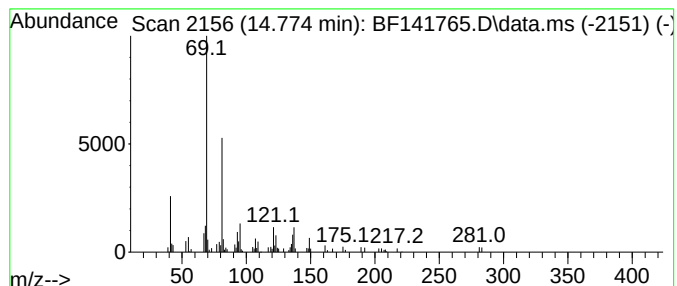
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	2.61 ng	57775	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
3			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	74
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141765.D
Acq On : 25 Feb 2025 15:35
Operator : RC/JU
Sample : Q1421-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-CLAY-CF02-01

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
2-Pentanone, 4-...	4.987	3.5	ng	71829	1	6.781	409394	20.0
Benzophenone	10.528	4.5	ng	135182	3	9.816	601858	20.0
n-Hexadecanoic ...	11.833	2.6	ng	71748	4	11.298	556798	20.0
Pentafluoroprop...	13.786	5.6	ng	113601	5	13.939	404524	20.0
9-Octadecenamid...	14.692	2.0	ng	44819	6	15.386	443457	20.0
Supraene	14.774	2.6	ng	57775	6	15.386	443457	20.0