LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140013.D
Acq On : 24 Oct 2024 21:04
Operator : RC/JU
Sample : P4467-01
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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	7	16	23	rBV	1230105	1991808	92.52%	11.462%
2	5.122	505	515	520	rBV2	13834	24672	1.15%	0.142%
3	5.504	574	580	585	rBV	1451549	1939136	90.07%	11.159%
4	6.504	744	750	756	rBV	1341610	1916176	89.01%	11.027%
5	6.887	810	815	820	rBV	392337	484883	22.52%	2.790%
6	7.445	904	910	915	rBV	987066	1295622	60.18%	7.456%
7	8.169	1028	1033	1038	rBV	506794	615484	28.59%	3.542%
8	9.245	1210	1216	1238	rBV	1679733	2152803	100.00%	12.389%
9	9.922	1326	1331	1344	rVB	524206	663815	30.83%	3.820%
10	10.634	1447	1452	1459	rBV	213126	266468	12.38%	1.533%
11	10.710	1460	1465	1477	rVV	975546	1230128	57.14%	7.079%
12	11.410	1579	1584	1591	rBV	469397	581805	27.03%	3.348%
13	11.475	1591	1595	1599	rVB	20620	24748	1.15%	0.142%
14	11.933	1667	1673	1686	rBV	163786	249215	11.58%	1.434%
15	12.716	1801	1806	1819	rBV	37217	63375	2.94%	0.365%
16	12.992	1848	1853	1859	rBV	1105146	1417860	65.86%	8.159%
17	13.733	1968	1979	1993	rBV	12160	55050	2.56%	0.317%
18	13.898	2001	2007	2023	rBV	46403	115600	5.37%	0.665%
19	14.045	2027	2032	2039	rVV	294048	387926	18.02%	2.232%
20	14.721	2127	2147	2163	rBV2	294877	1409048	65.45%	8.109%
21	15.527	2277	2284	2298	rBV	300461	491486	22.83%	2.828%

Sum of corrected areas: 17377108

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
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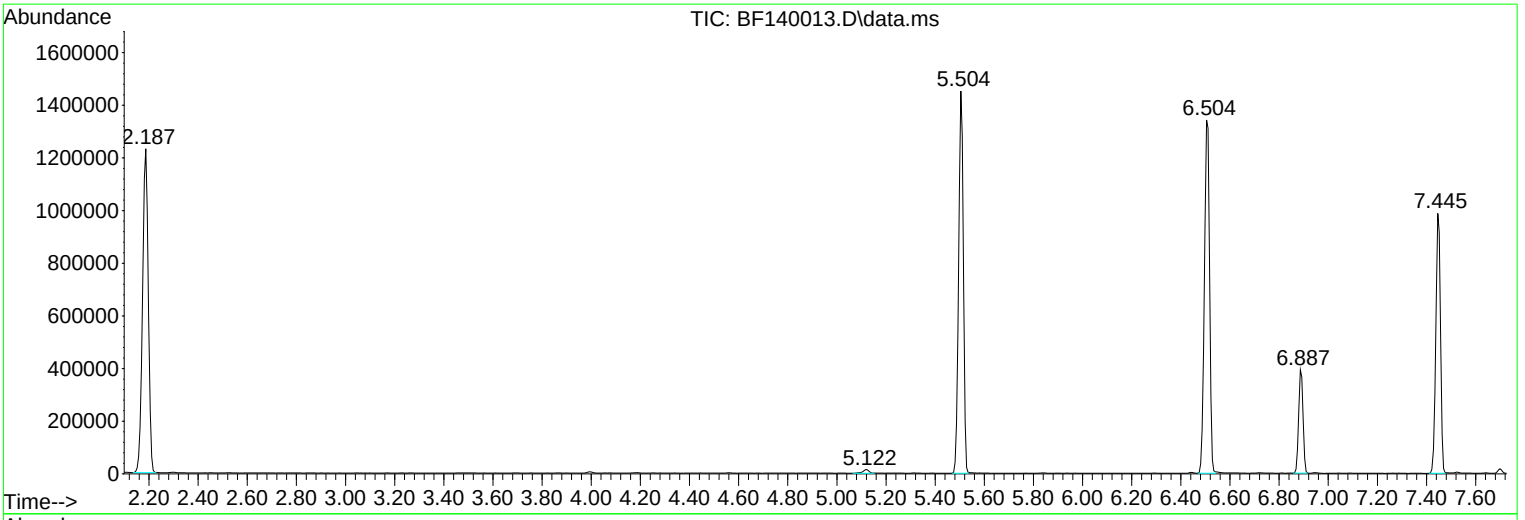
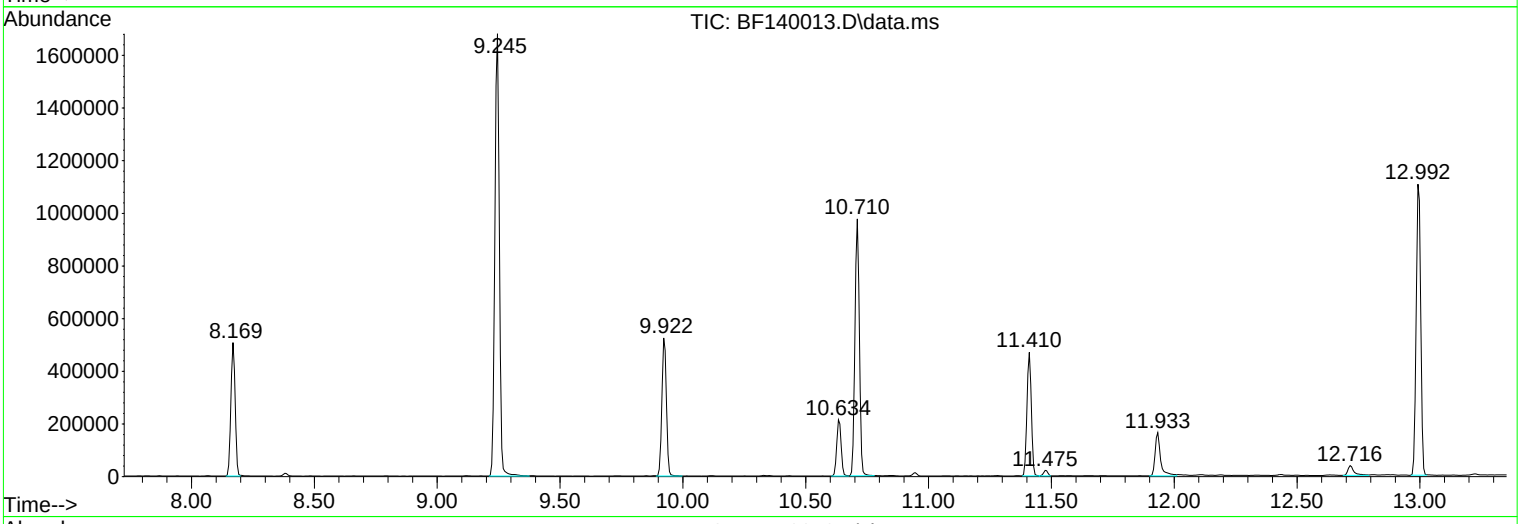
Misc :
ALS Vial : 14 Sample Multiplier: 1

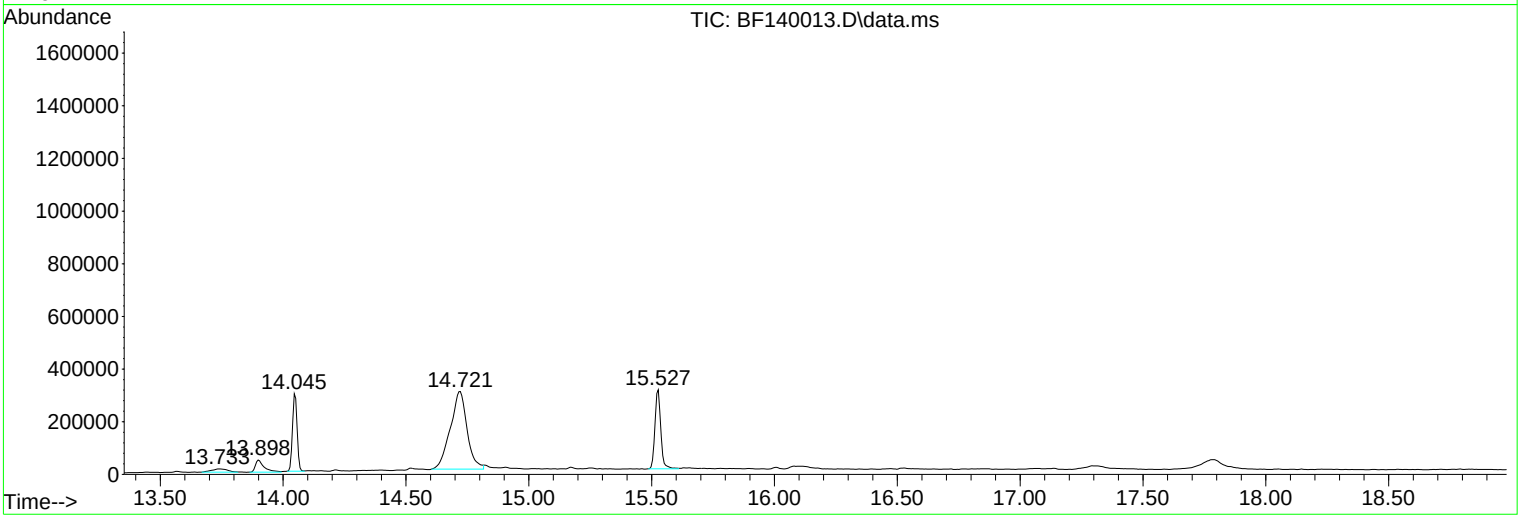
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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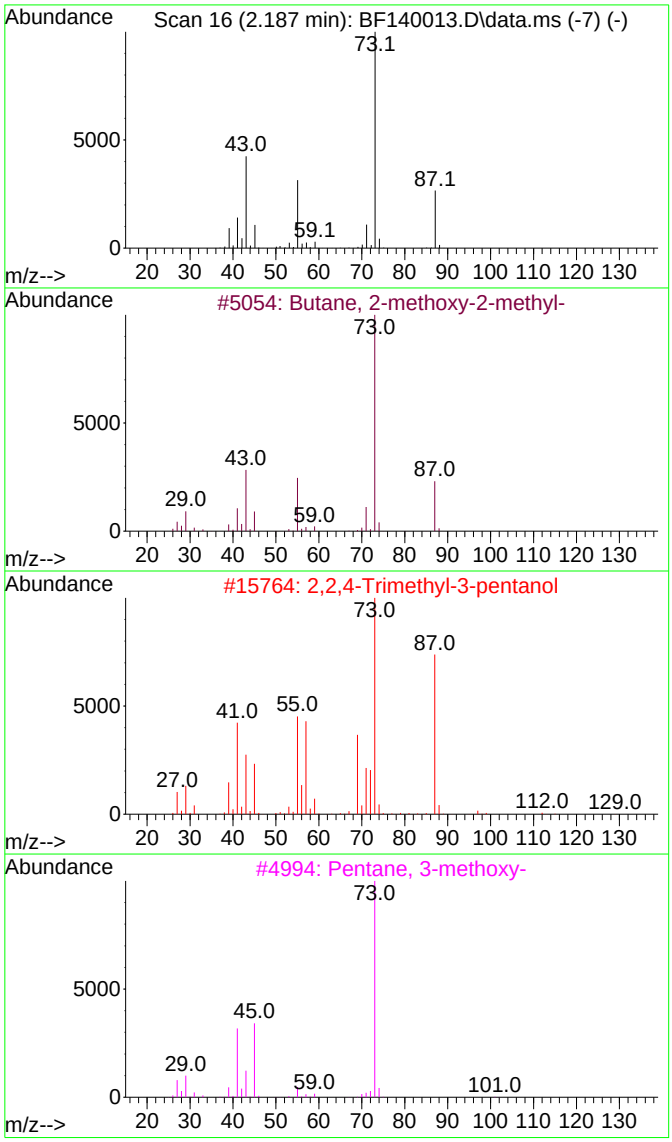
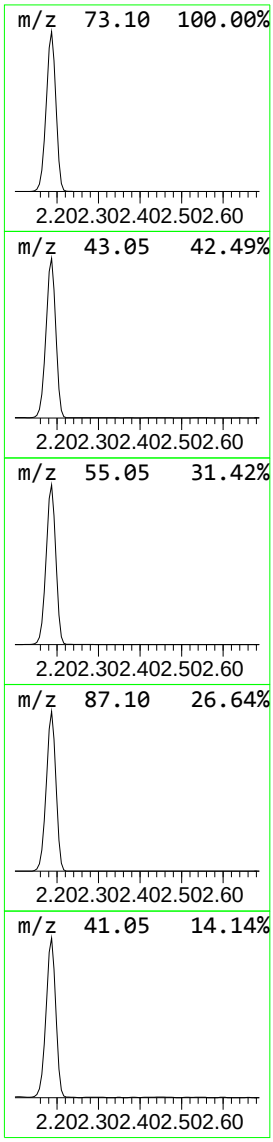
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	82.16 ng	1991810	1,4-Dichlorobenzene-d4	6.887

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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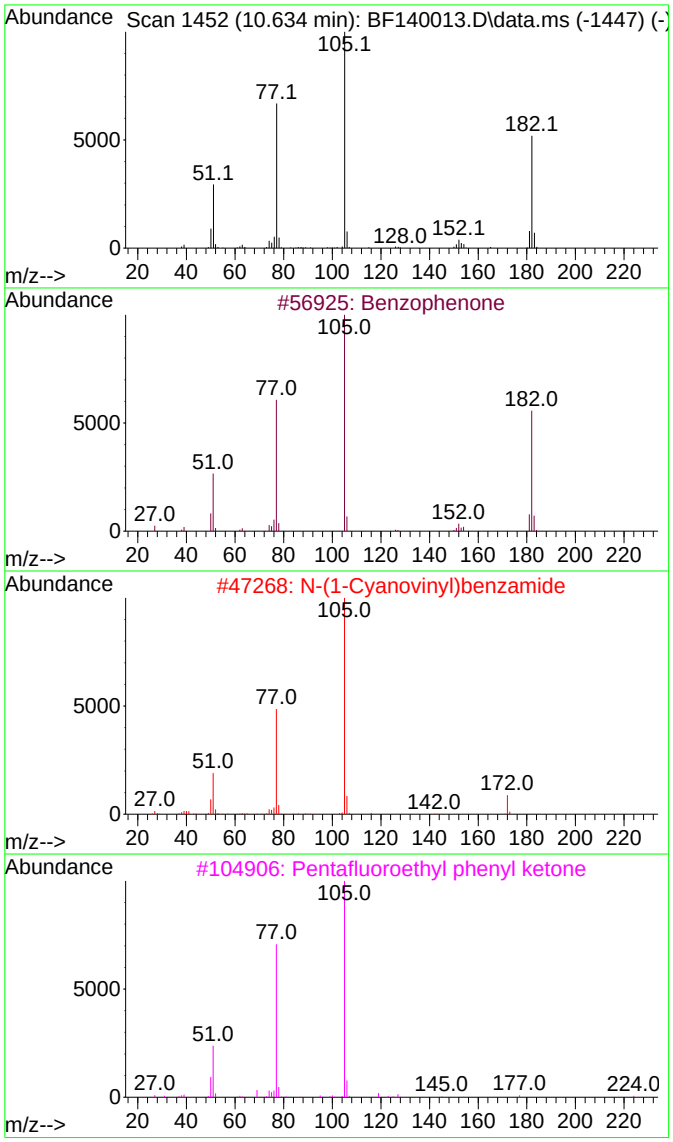
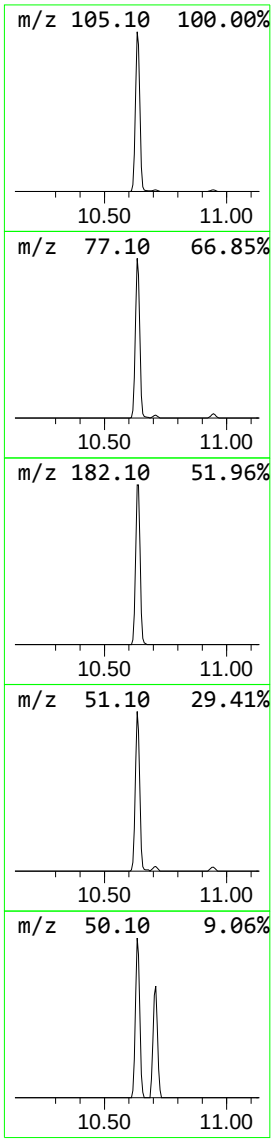
Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	8.03 ng	266468	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	50
3	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140013.D
Acq On : 24 Oct 2024 21:04
Operator : RC/JU
Sample : P4467-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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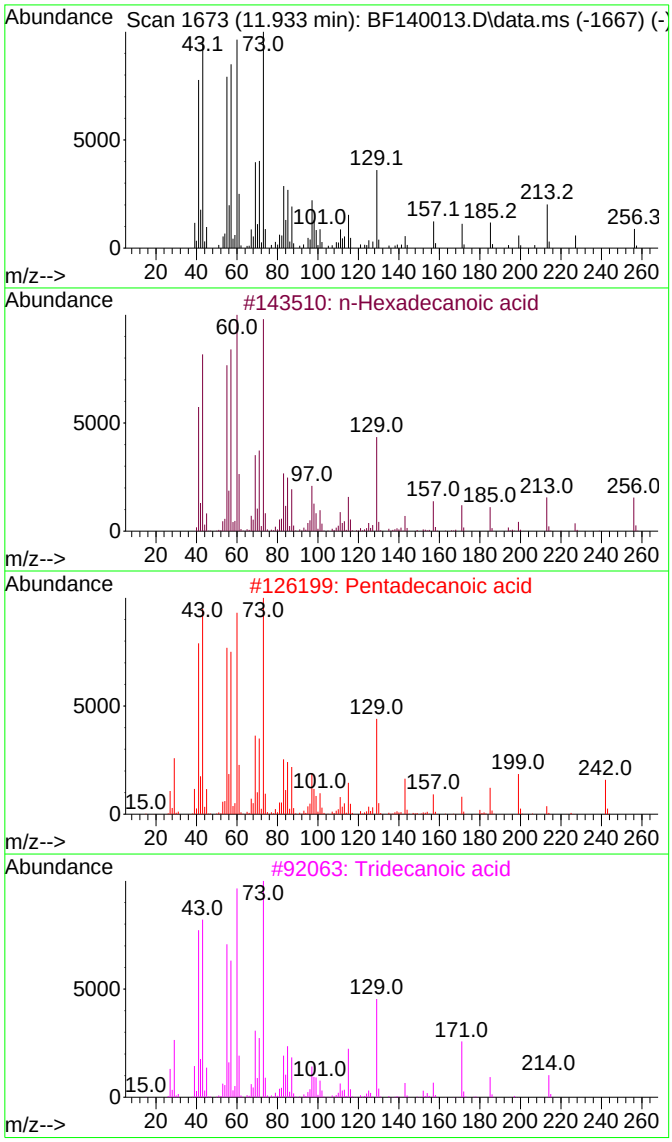
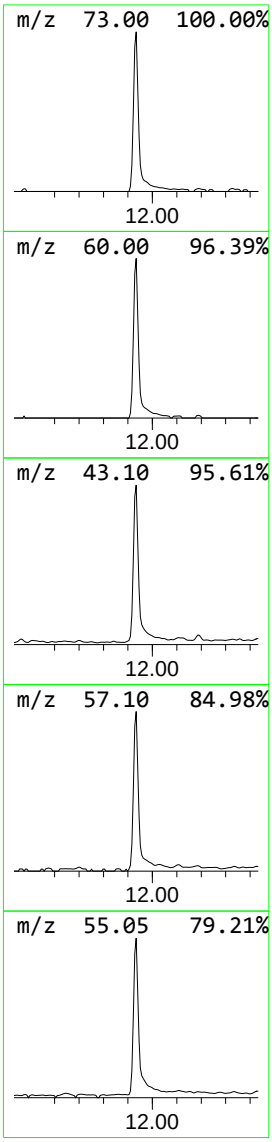
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	8.57 ng	249215	Phenanthrene-d10	11.410

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Data File : BF140013.D
Acq On : 24 Oct 2024 21:04
Operator : RC/JU
Sample : P4467-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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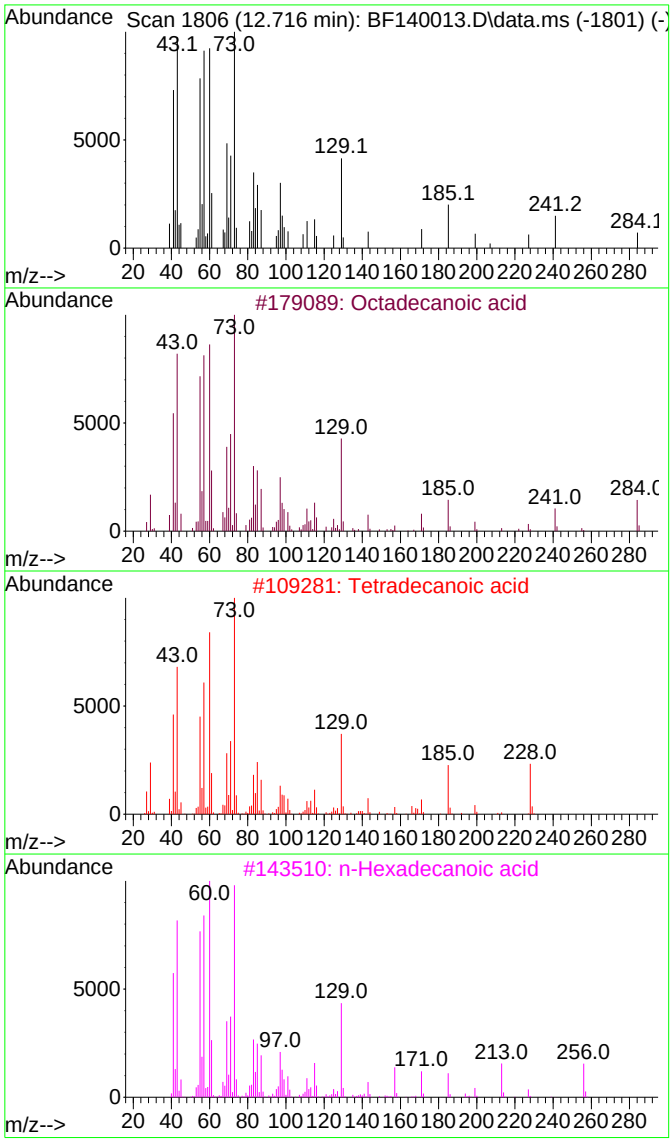
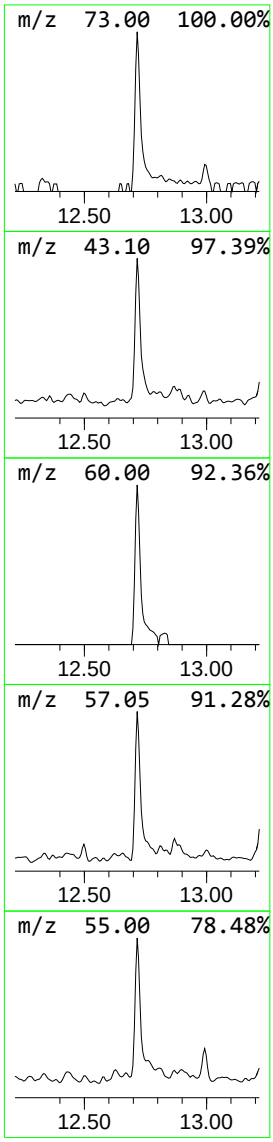
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.18 ng	63375	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
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Acq On : 24 Oct 2024 21:04
Operator : RC/JU
Sample : P4467-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
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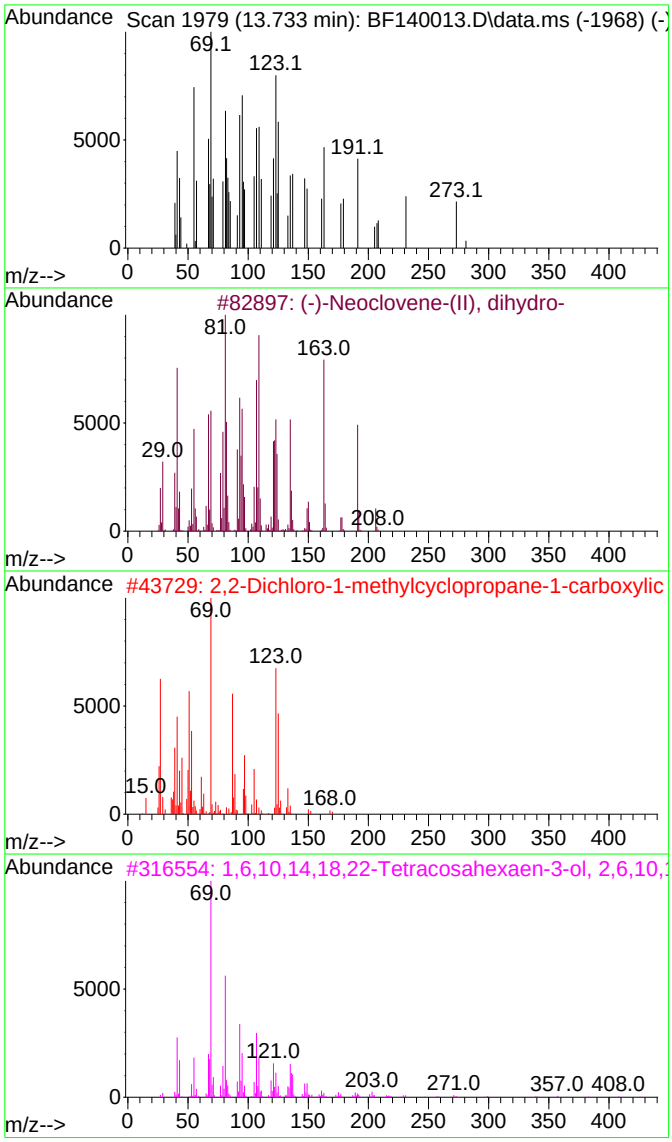
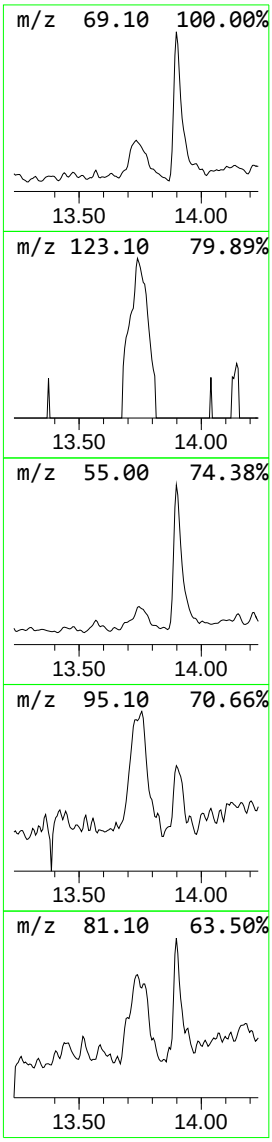
Peak Number 5 unknown13.733 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	2.84 ng	55050	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	38
2	2,2-Dichloro-1-methylcyclopropan...	168	C5H6Cl2O2	001447-14-9	35
3	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	097232-74-1	27
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	27
5	3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	27





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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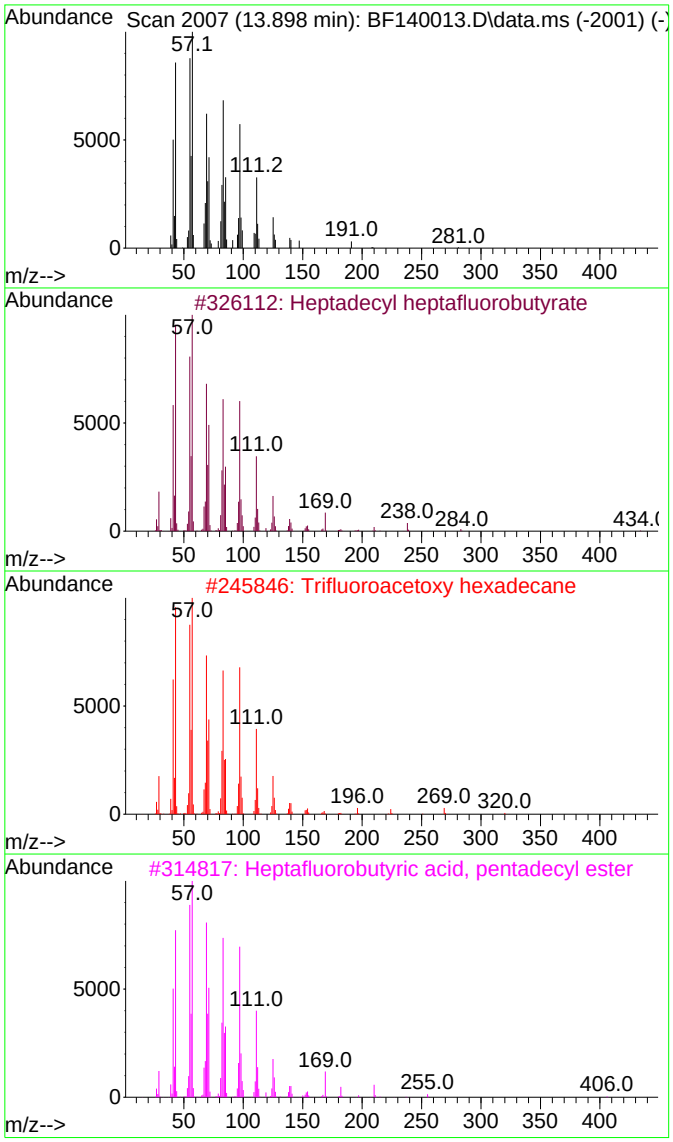
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

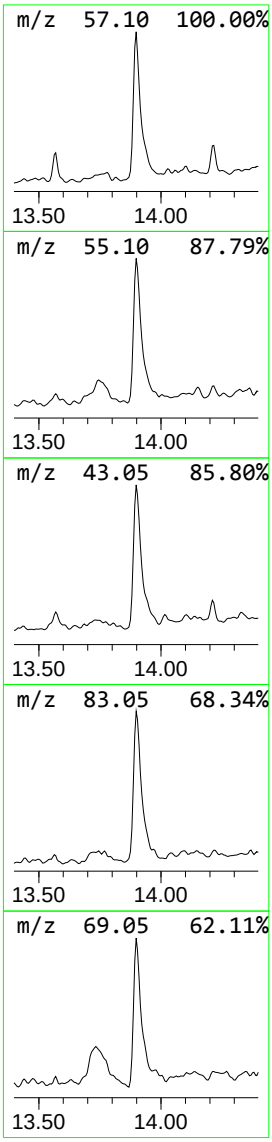
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.96 ng	115600	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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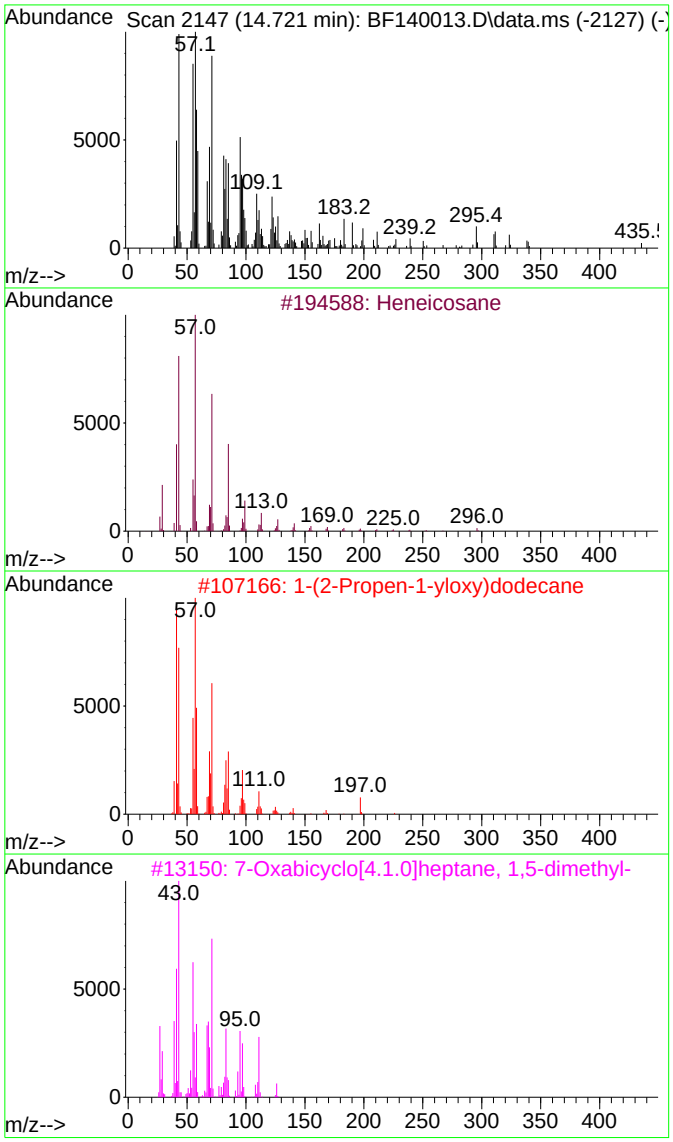
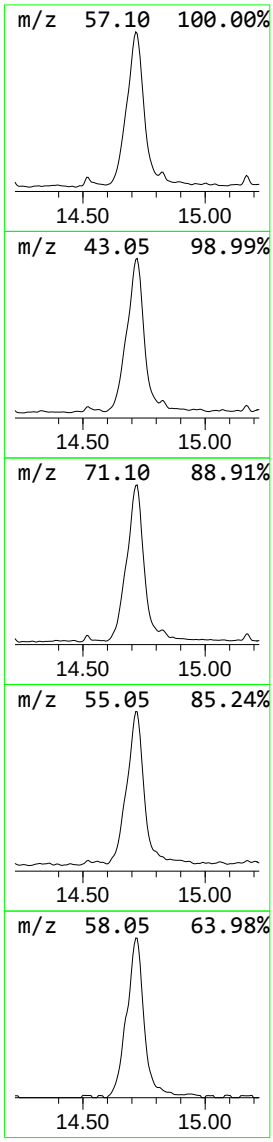
Peak Number 7 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.722	72.65 ng	1409050	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	74
2	1-(2-Propen-1-yloxy)dodecane	226	C15H30O	006145-80-8	60
3	7-Oxabicyclo[4.1.0]heptane, 1,5-...	126	C8H14O	162239-52-3	49
4	Acetamide, 2-(2-thiophenyl)-N-et...	295	C17H29NOS	1010415-41-7	46
5	2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	46





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.187	82.2	ng	1991810	1	6.887	484883	20.0
Benzophenone	10.634	8.0	ng	266468	3	9.922	663815	20.0
n-Hexadecanoic ...	11.933	8.6	ng	249215	4	11.410	581805	20.0
Octadecanoic acid	12.716	2.2	ng	63375	4	11.410	581805	20.0
unknown13.733	13.733	2.8	ng	55050	5	14.045	387926	20.0
Heptadecyl hept...	13.898	6.0	ng	115600	5	14.045	387926	20.0
Heneicosane	14.722	72.7	ng	1409050	5	14.045	387926	20.0