LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140045.D
Acq On : 25 Oct 2024 18:50
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

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: BF140045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	9	17	24	rVB	539503	850169	32.95%	4.389%
2	5.116	508	514	520	rVB2	20306	31220	1.21%	0.161%
3	5.504	574	580	585	rBV	1669403	2203233	85.39%	11.375%
4	5.628	596	601	608	rVB	23123	37348	1.45%	0.193%
5	5.993	658	663	670	rBV	73802	109348	4.24%	0.565%
6	6.122	677	685	694	rVB2	18282	40494	1.57%	0.209%
7	6.269	706	710	711	rBV	37541	46144	1.79%	0.238%
8	6.287	711	713	718	rVB	49615	57666	2.24%	0.298%
9	6.504	744	750	768	rVB	1620264	2306553	89.40%	11.909%
10	6.887	810	815	820	rBV	518904	634030	24.57%	3.273%
11	7.445	904	910	915	rBV	1147579	1510443	58.54%	7.798%
12	7.698	948	953	959	rBV	77505	93831	3.64%	0.484%
13	8.169	1027	1033	1038	rBV	664657	828760	32.12%	4.279%
14	8.381	1064	1069	1076	rVB2	34466	46562	1.80%	0.240%
15	9.245	1210	1216	1226	rBV	1995908	2580057	100.00%	13.321%
16	9.922	1326	1331	1345	rVB	662990	869368	33.70%	4.489%
17	10.639	1447	1453	1460	rBV	516347	669821	25.96%	3.458%
18	10.710	1460	1465	1479	rVV	1090375	1415199	54.85%	7.307%
19	10.828	1480	1485	1493	rVB2	17549	31555	1.22%	0.163%
20	10.945	1500	1505	1511	rVB	68132	82752	3.21%	0.427%
21	11.410	1579	1584	1589	rBV	582769	717913	27.83%	3.707%
22	11.933	1667	1673	1687	rBV	322907	491569	19.05%	2.538%
23	12.716	1802	1806	1815	rBV	57600	103940	4.03%	0.537%
24	12.816	1819	1823	1827	rVV	21667	27765	1.08%	0.143%
25	12.998	1848	1854	1862	rBV	1354836	1816148	70.39%	9.377%
26	13.222	1889	1892	1896	rVB	23528	31096	1.21%	0.161%
27	13.569	1947	1951	1958	rVB	29785	52246	2.02%	0.270%
28	13.892	2002	2006	2021	rBV	122548	243105	9.42%	1.255%
29	14.051	2028	2033	2039	rVB	419104	555316	21.52%	2.867%
30	14.210	2057	2060	2068	rVB	33657	48189	1.87%	0.249%
31	14.516	2109	2112	2117	rBV	33602	44856	1.74%	0.232%
32	14.810	2157	2162	2171	rBV2	118839	234545	9.09%	1.211%
33	14.904	2175	2178	2183	rVB	54804	71417	2.77%	0.369%
34	15.527	2279	2284	2299	rVB	281160	486014	18.84%	2.509%

Sum of corrected areas: 19368672

Instrument :
BNA_F
ClientSampleId :
BP-B5

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
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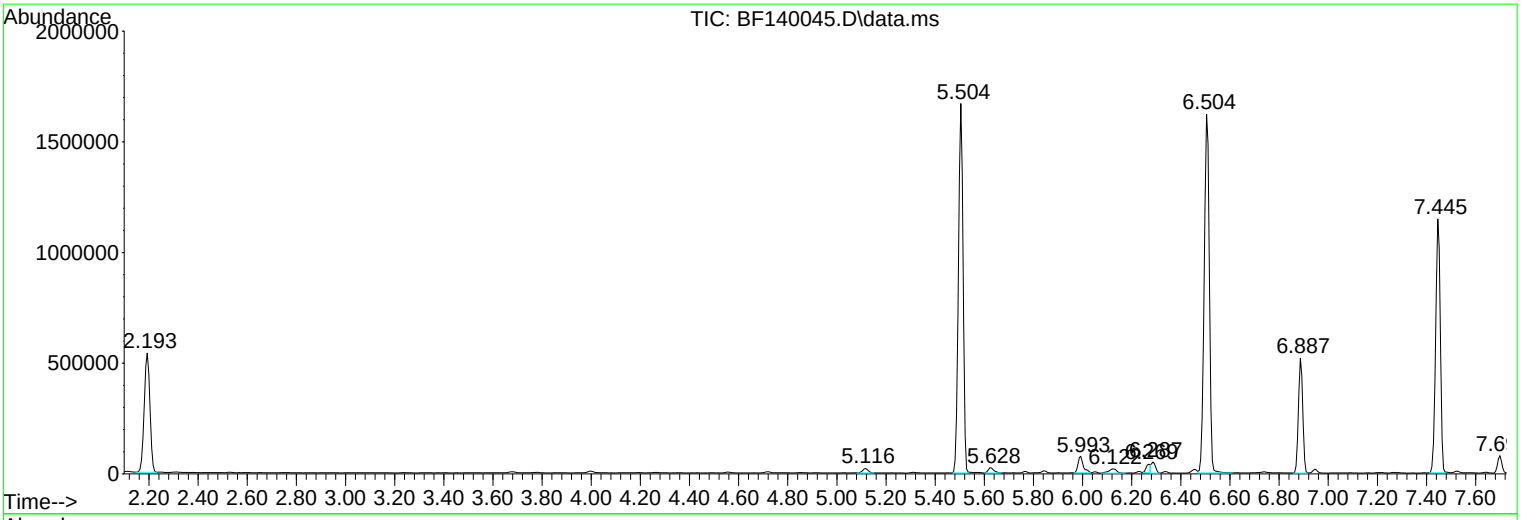
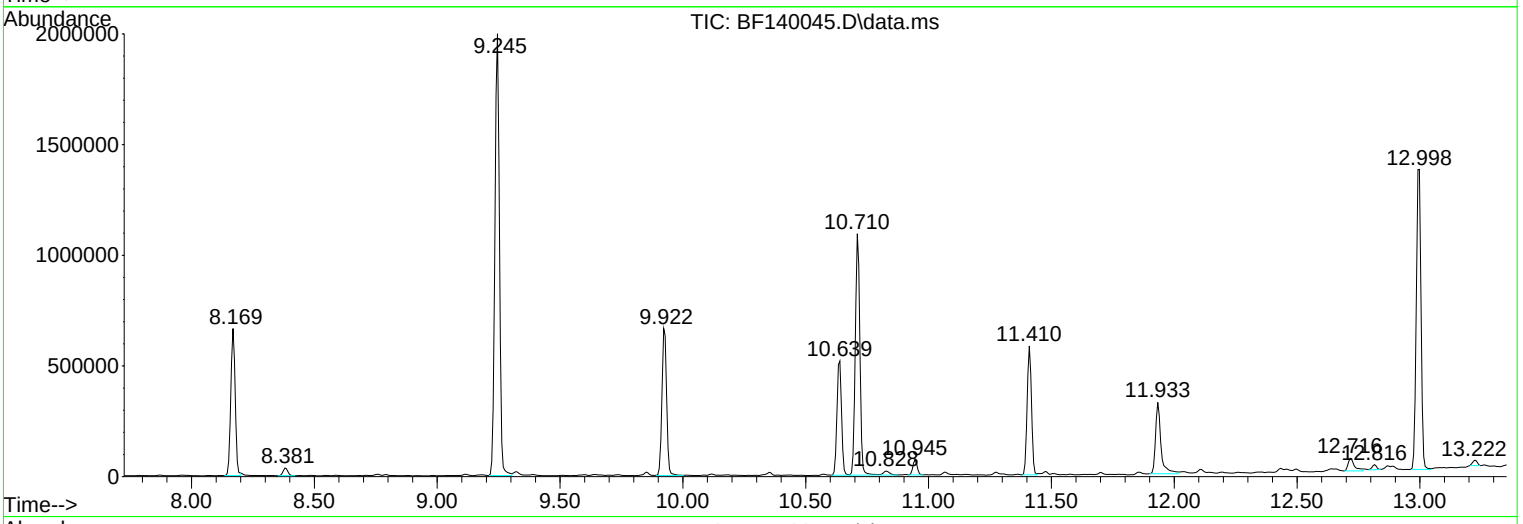
Misc :
ALS Vial : 21 Sample Multiplier: 1

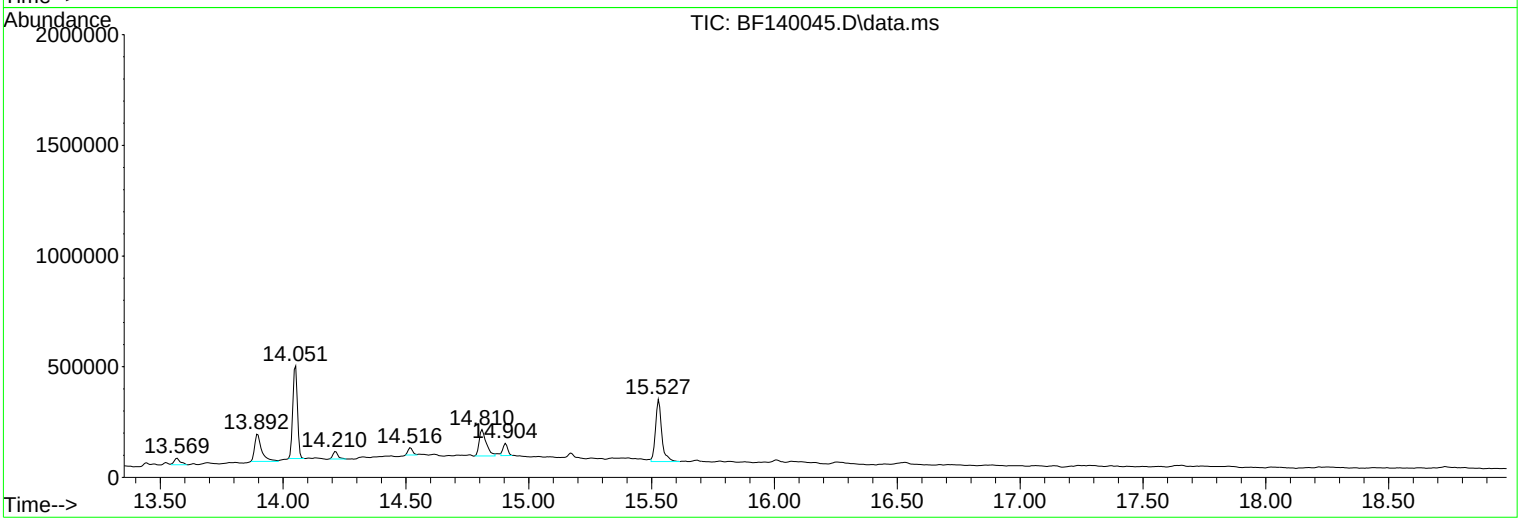
Instrument :
BNA_F
ClientSampleId :
BP-B5

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
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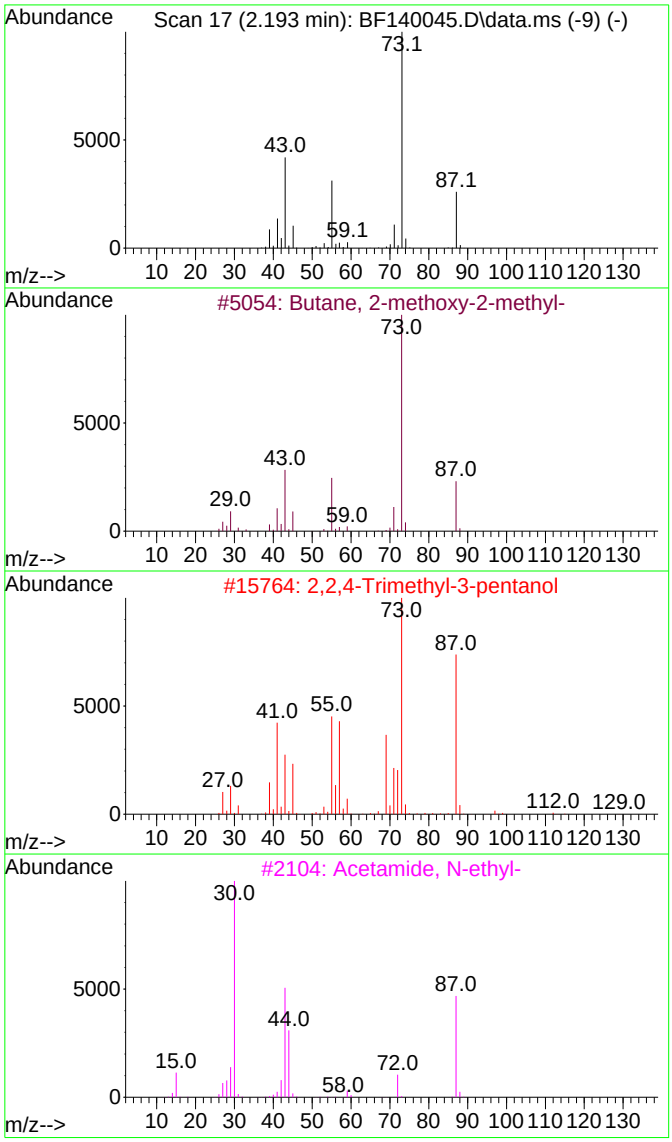
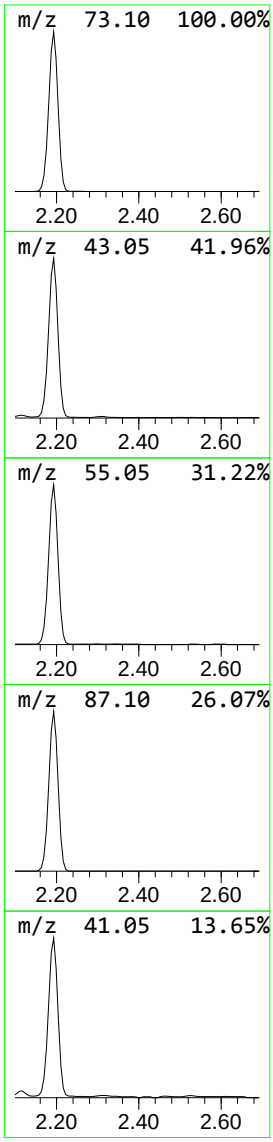
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	26.82 ng	850169	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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Operator : RC/JU
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Misc :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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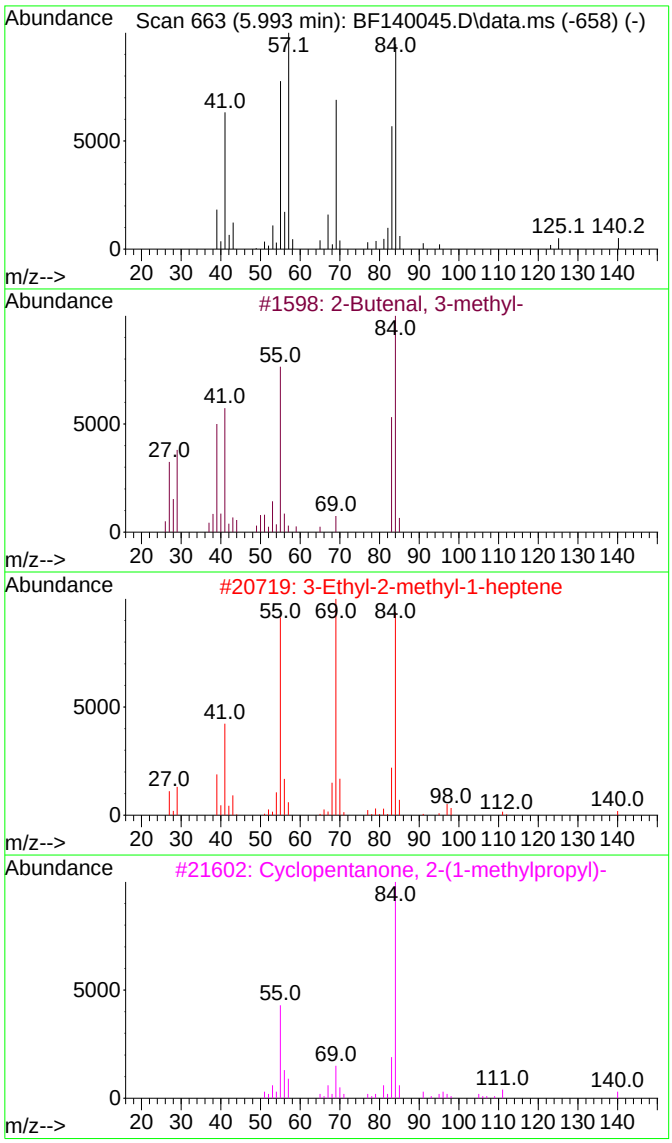
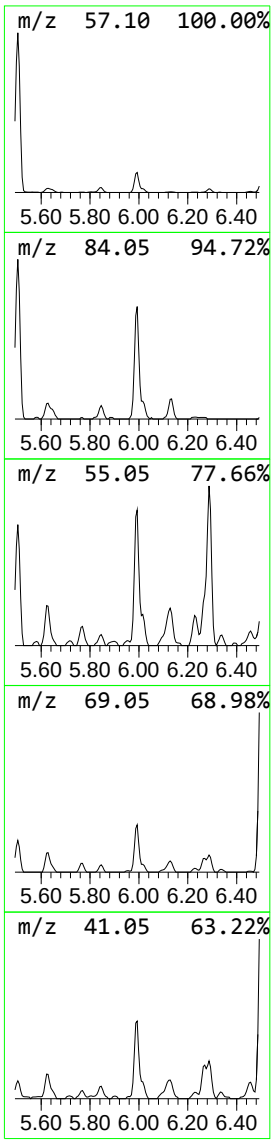
****

Peak Number 2 2-Butenal, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.993	3.45 ng	109348	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	53
2	3-Ethyl-2-methyl-1-heptene	140	C10H20	019780-60-0	47
3	Cyclopentanone, 2-(1-methylpropyl)-	140	C9H16O	006376-92-7	47
4	Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	45
5	3-Hexene	84	C6H12	000592-47-2	43





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Acq On : 25 Oct 2024 18:50
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

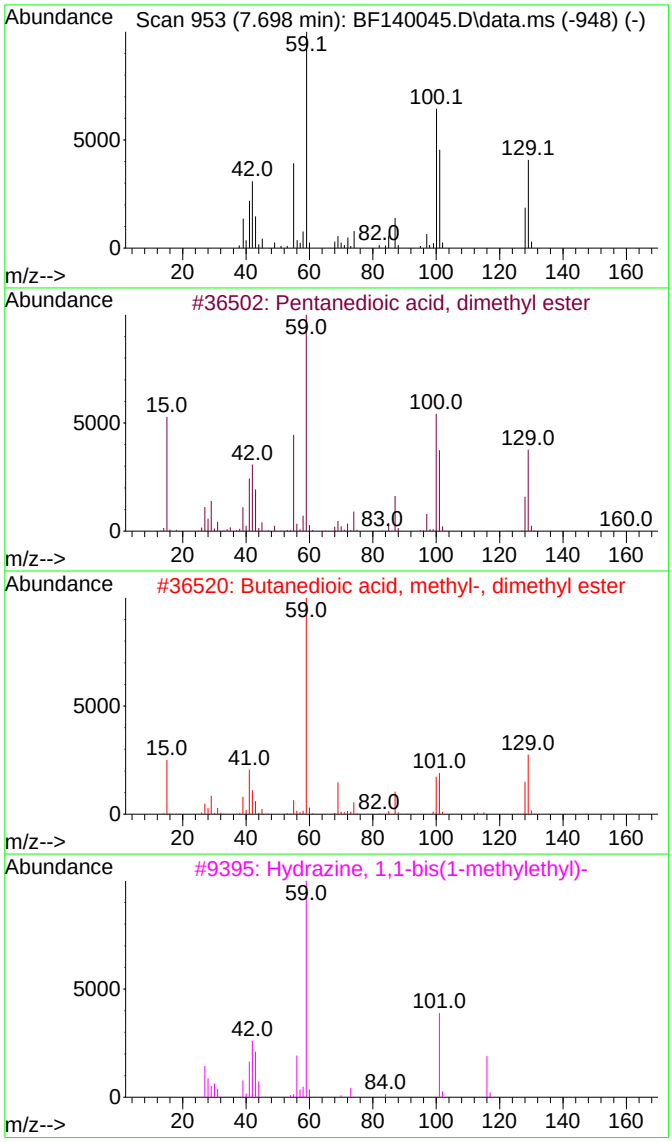
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

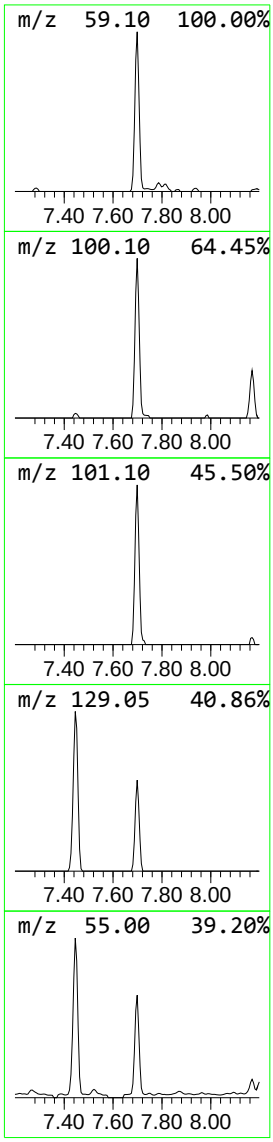
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.26 ng	93831	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	90
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	40
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
4	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	22
5	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	17





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Instrument :
BNA_F
ClientSampleId :
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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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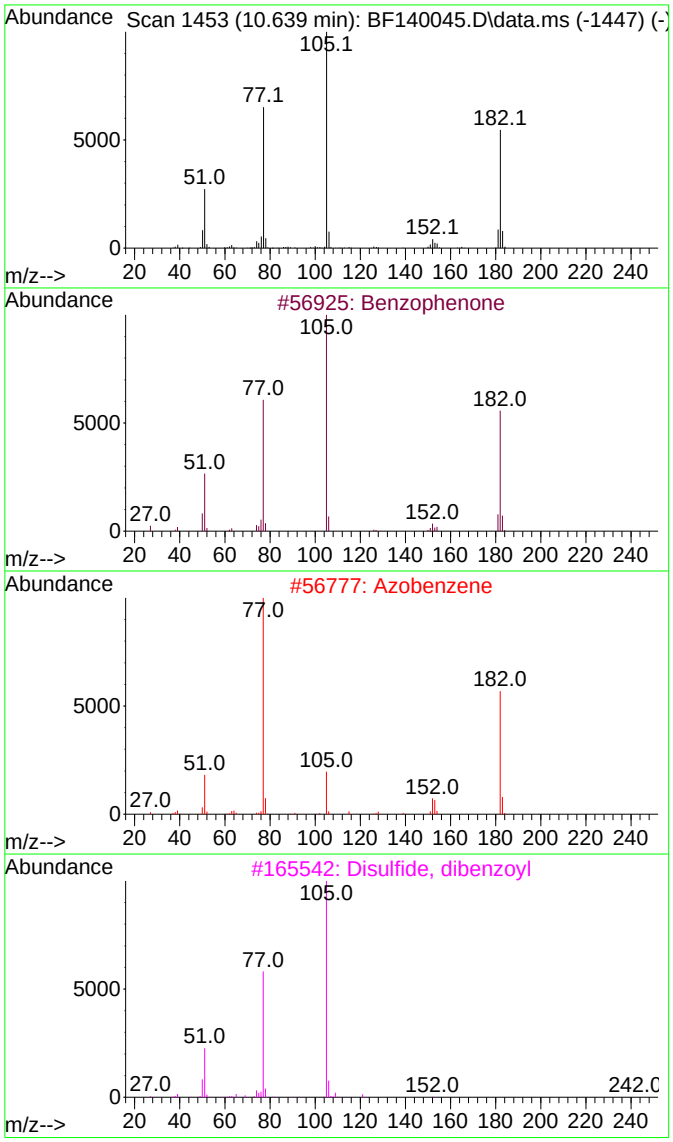
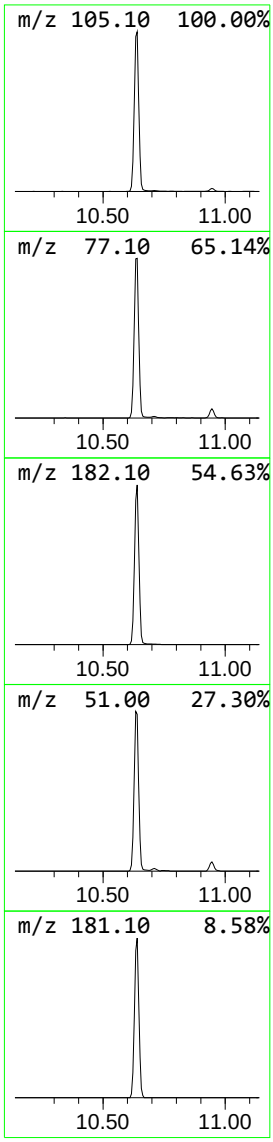
****

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	15.41 ng	669821	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47





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Instrument :
BNA_F
ClientSampleId :
BP-B5

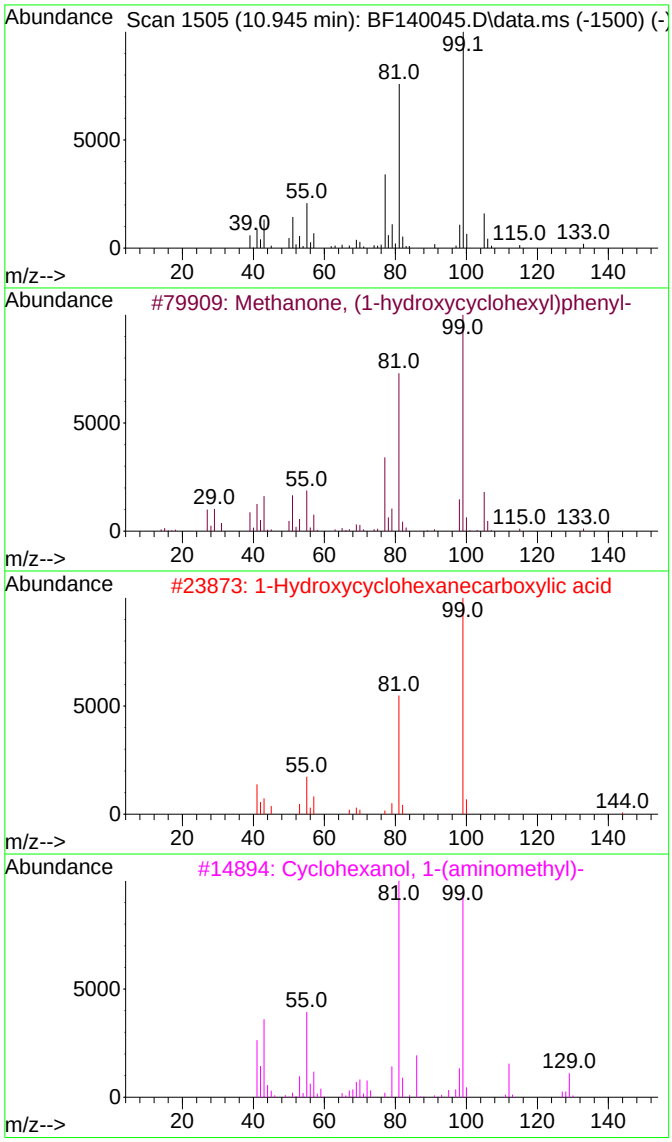
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

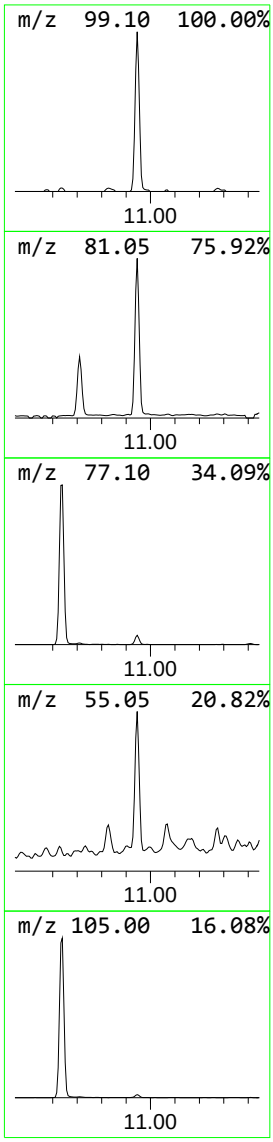
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Methanone, (1-hydroxycycloh... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	2.31 ng	82752	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
3	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
4	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	45
5	1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	36





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BP-B5

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TIC Library : C:\Database\NIST20.L
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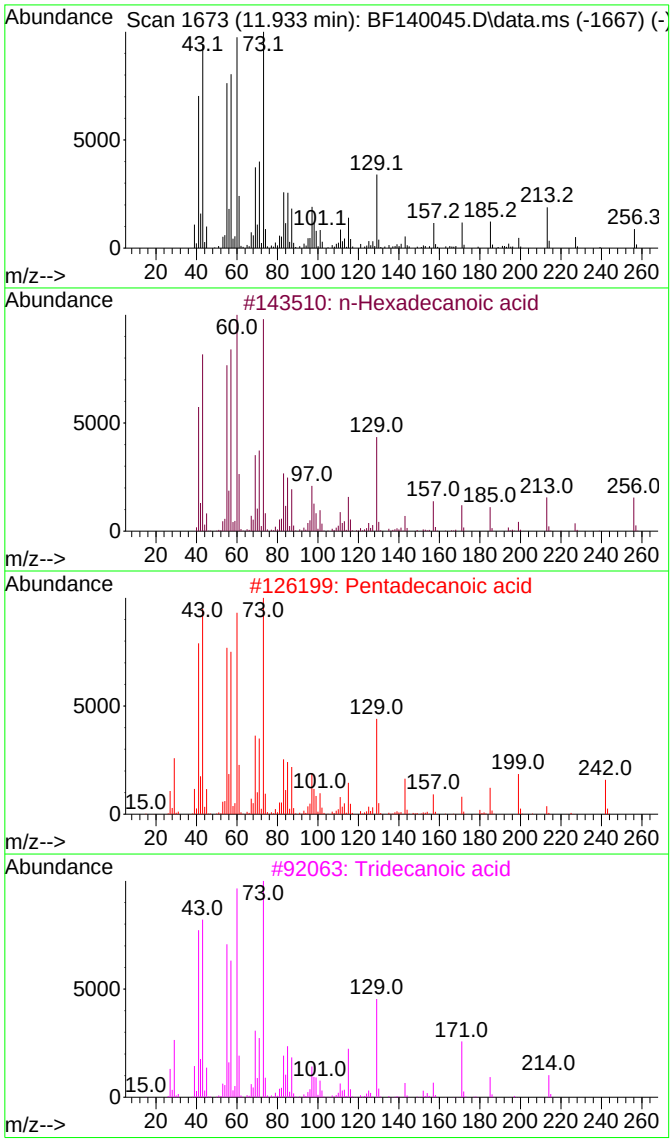
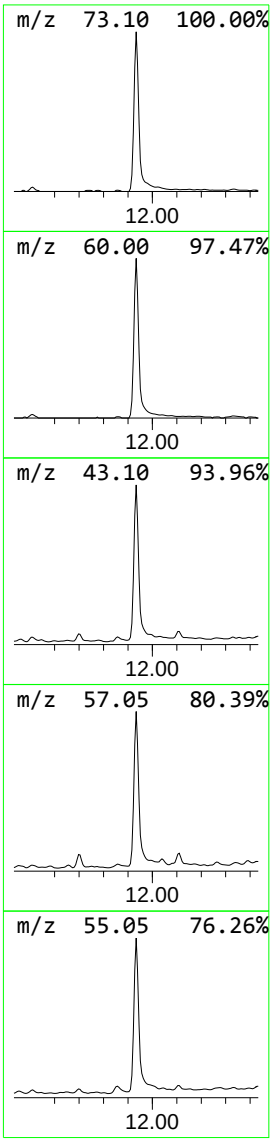
Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	13.69 ng	491569	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	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78





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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

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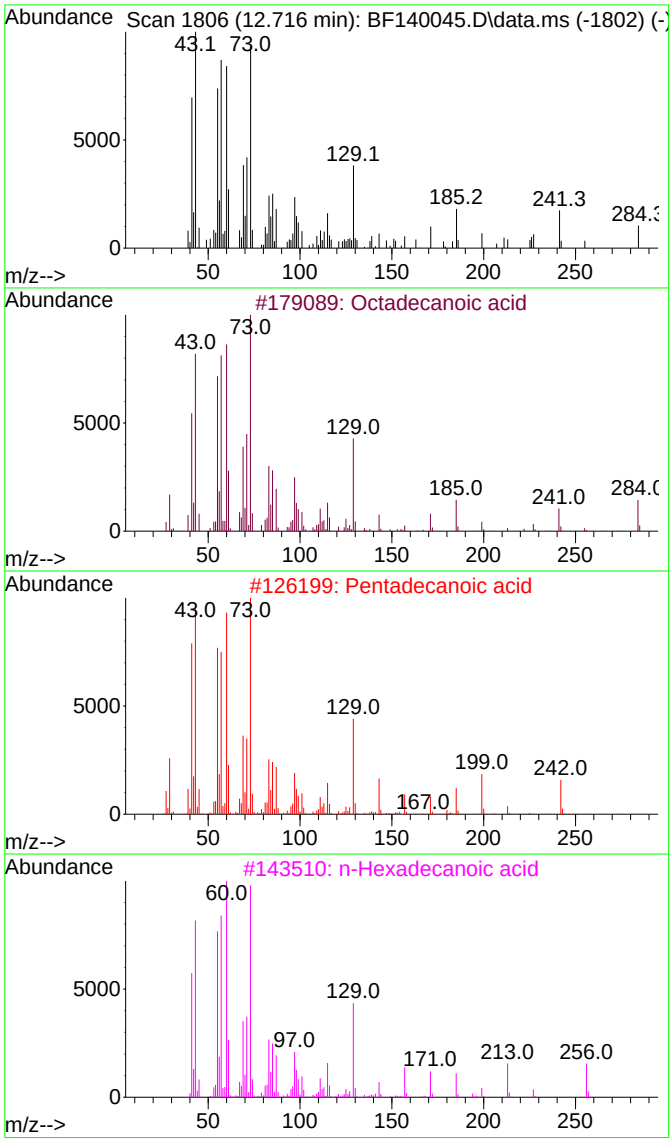
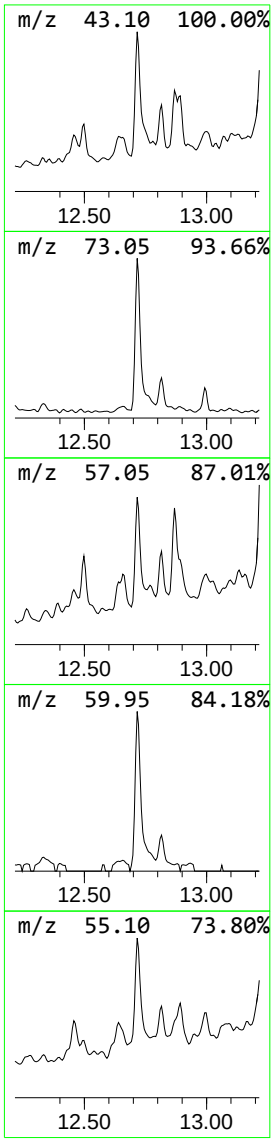
Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.90 ng	103940	Phenanthrene-d10	11.410

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	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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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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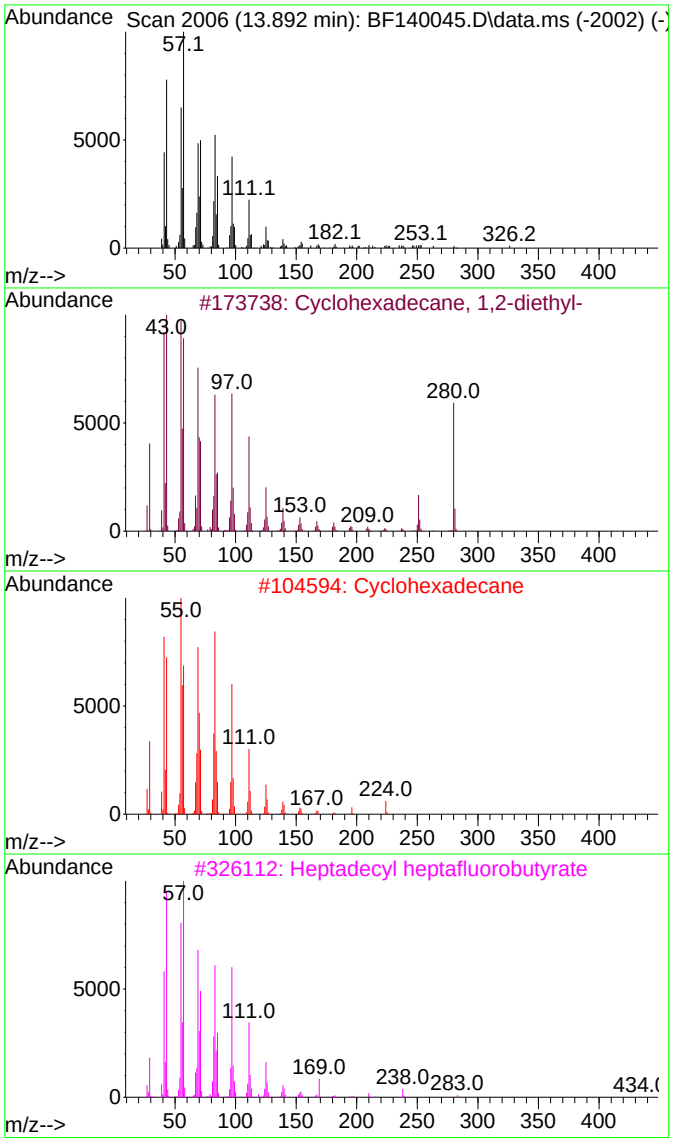
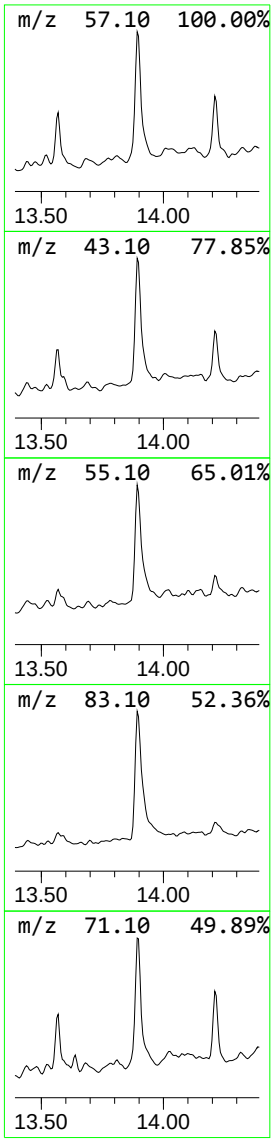
Peak Number 8 Cyclohexadecane, 1,2-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	8.76 ng	243105	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	97
2	Cyclohexadecane	224	C16H32	000295-65-8	96
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91





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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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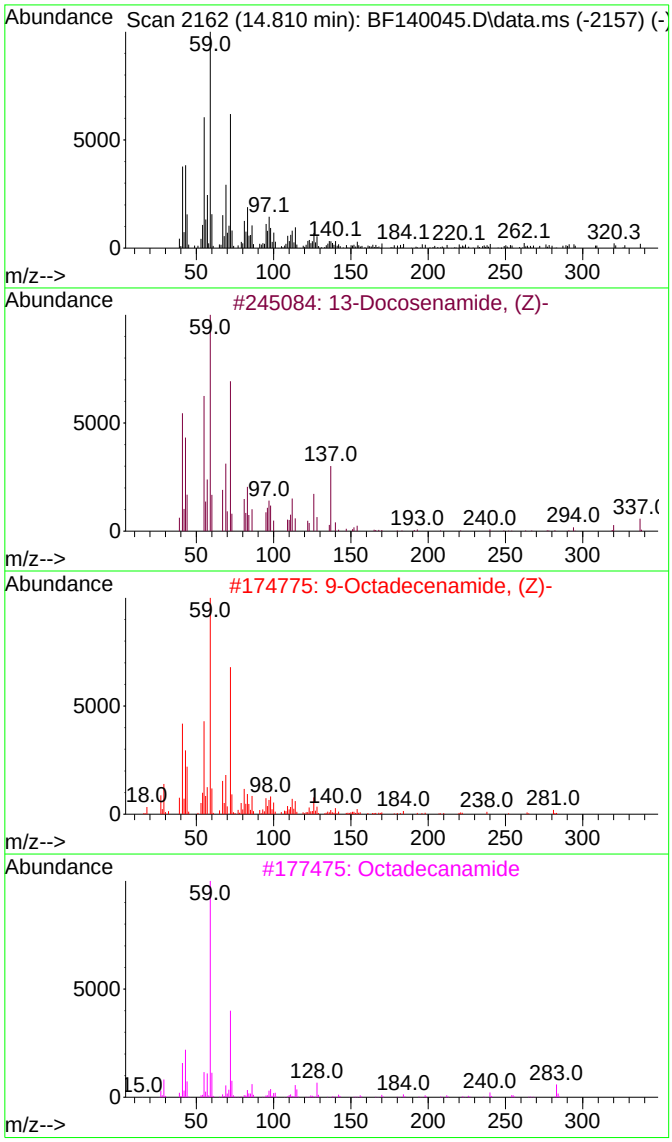
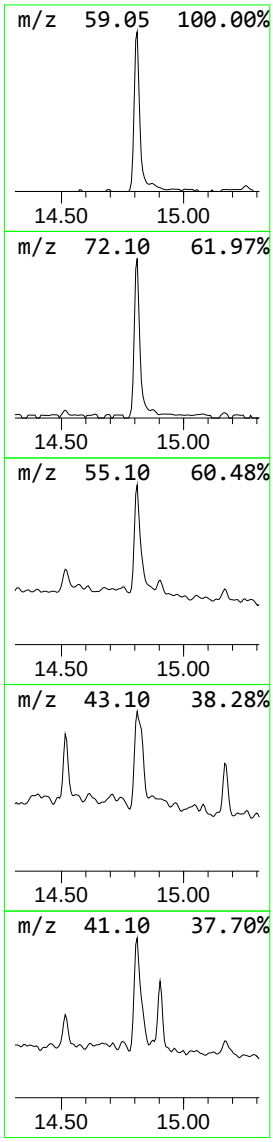
Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	9.65 ng	234545	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Octadecanamide	283	C18H37NO	000124-26-5	53
4	d-Glucosamine	179	C6H13NO5	000090-77-7	53
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140045.D
Acq On : 25 Oct 2024 18:50
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

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

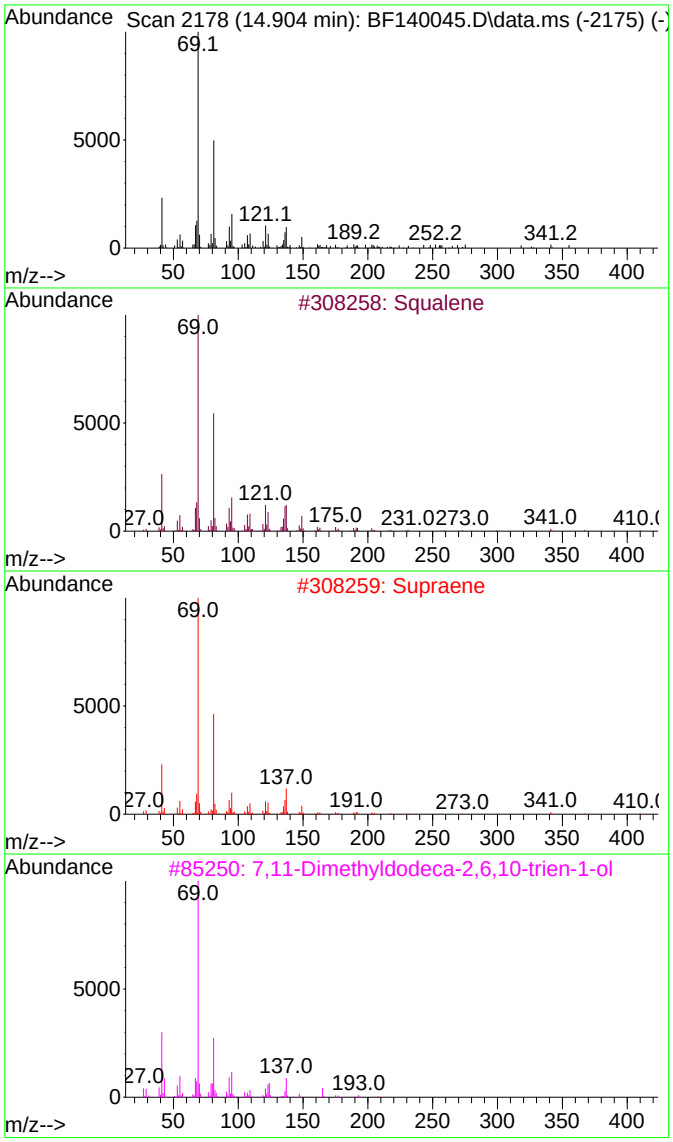
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

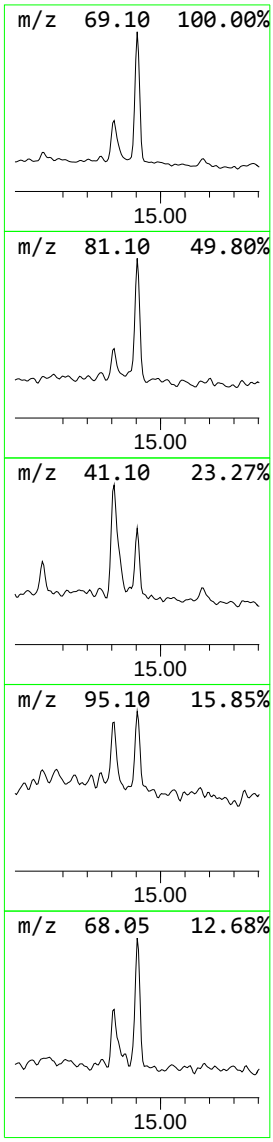
****

Peak Number 10 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.94 ng	71417	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59
5	Cyclopropanecarboxylic acid, 4-i...	204	C13H16O2	1000331-01-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140045.D
Acq On : 25 Oct 2024 18:50
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.193	26.8	ng	850169	1	6.887	634030	20.0
2-Butenal, 3-me...	5.993	3.5	ng	109348	1	6.887	634030	20.0
Pentanedioic ac...	7.698	2.3	ng	93831	2	8.169	828760	20.0
Benzophenone	10.639	15.4	ng	669821	3	9.922	869368	20.0
Methanone, (1-h...	10.945	2.3	ng	82752	4	11.410	717913	20.0
n-Hexadecanoic ...	11.933	13.7	ng	491569	4	11.410	717913	20.0
Octadecanoic acid	12.716	2.9	ng	103940	4	11.410	717913	20.0
Cyclohexadecane...	13.892	8.8	ng	243105	5	14.051	555316	20.0
13-Docosenamide...	14.810	9.7	ng	234545	6	15.527	486014	20.0
Squalene	14.904	2.9	ng	71417	6	15.527	486014	20.0