LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123060.D
Acq On : 28 Jan 2021 15:30
Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0014-048-COMP-G

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	7	15	21	rBV	623928	790365	8.79%	1.288%
2	5.504	576	581	585	rBV	4613441	4867015	54.13%	7.933%
3	6.510	747	752	768	rBV	4632844	5179165	57.60%	8.442%
4	6.893	813	817	820	rBV	1903517	1523284	16.94%	2.483%
5	7.045	839	843	847	rVB	3119221	2794306	31.07%	4.555%
6	7.451	907	912	915	rBV	4590911	5031996	55.96%	8.202%
7	8.175	1031	1035	1038	rBV	2394315	2003279	22.28%	3.265%
8	9.257	1213	1219	1222	rBV	7886430	7930051	88.19%	12.926%
9	9.645	1281	1285	1289	rBV	156862	132828	1.48%	0.217%
10	9.933	1330	1334	1338	rBV	2776781	2384100	26.51%	3.886%
11	10.722	1463	1468	1472	rBV	3985182	4000379	44.49%	6.521%
12	11.286	1559	1564	1568	rBV3	113884	150003	1.67%	0.245%
13	11.428	1583	1588	1590	rBV	2804960	2559761	28.47%	4.173%
14	11.445	1590	1591	1594	rVV	337537	250838	2.79%	0.409%
15	11.498	1597	1600	1604	rVB2	98722	100090	1.11%	0.163%
16	11.957	1674	1678	1682	rVV	1034841	905280	10.07%	1.476%
17	12.039	1689	1692	1694	rBV2	91203	92431	1.03%	0.151%
18	12.251	1725	1728	1732	rVB	102797	129136	1.44%	0.210%
19	12.410	1752	1755	1759	rBV	696236	647441	7.20%	1.055%
20	12.469	1762	1765	1770	rVV2	192057	236720	2.63%	0.386%
21	12.510	1770	1772	1779	rVB3	79642	109841	1.22%	0.179%
22	12.645	1791	1795	1797	rBV	438786	370863	4.12%	0.605%
23	12.739	1808	1811	1817	rBV2	327209	345849	3.85%	0.564%
24	12.816	1821	1824	1826	rVV	177248	150023	1.67%	0.245%
25	12.869	1826	1833	1836	rVB	453784	501989	5.58%	0.818%
26	13.022	1852	1859	1862	rBV	8339260	8992146	100.00%	14.658%
27	13.174	1881	1885	1887	rBV2	109636	112881	1.26%	0.184%
28	13.204	1887	1890	1895	rVB3	87469	97677	1.09%	0.159%
29	13.269	1895	1901	1904	rVB3	71704	98758	1.10%	0.161%
30	13.310	1904	1908	1910	rBV2	88723	106236	1.18%	0.173%
31	13.498	1937	1940	1944	rBV	235891	218985	2.44%	0.357%
32	13.639	1961	1964	1968	rBV	723267	639820	7.12%	1.043%
33	13.674	1968	1970	1973	rBV	124627	115118	1.28%	0.188%
34	13.927	2008	2013	2022	rBV2	417293	752683	8.37%	1.227%
35	14.074	2033	2038	2041	rBV	2931771	2993956	33.30%	4.880%
36	14.098	2041	2042	2048	rVB	266124	207135	2.30%	0.338%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123060.D
Acq On : 28 Jan 2021 15:30
Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0014-048-COMP-G

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.392	2088	2092	2096	rVB	158602	148016	1.65%	0.241%
38	14.551	2113	2119	2122	rBV4	105626	165415	1.84%	0.270%
39	15.121	2212	2216	2220	rBV	147838	251895	2.80%	0.411%
40	15.210	2228	2231	2234	rBV	94921	107152	1.19%	0.175%
41	15.427	2265	2268	2275	rVB	101534	131037	1.46%	0.214%
42	15.492	2275	2279	2284	rBV	151991	182599	2.03%	0.298%
43	15.563	2285	2291	2295	rVV	1964258	2503977	27.85%	4.082%
44	15.598	2295	2297	2303	rVB3	98400	134018	1.49%	0.218%
45	16.051	2370	2374	2379	rBV	68725	102686	1.14%	0.167%
46	16.574	2459	2463	2473	rVB2	49930	98693	1.10%	0.161%

Sum of corrected areas: 61347916

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Instrument :
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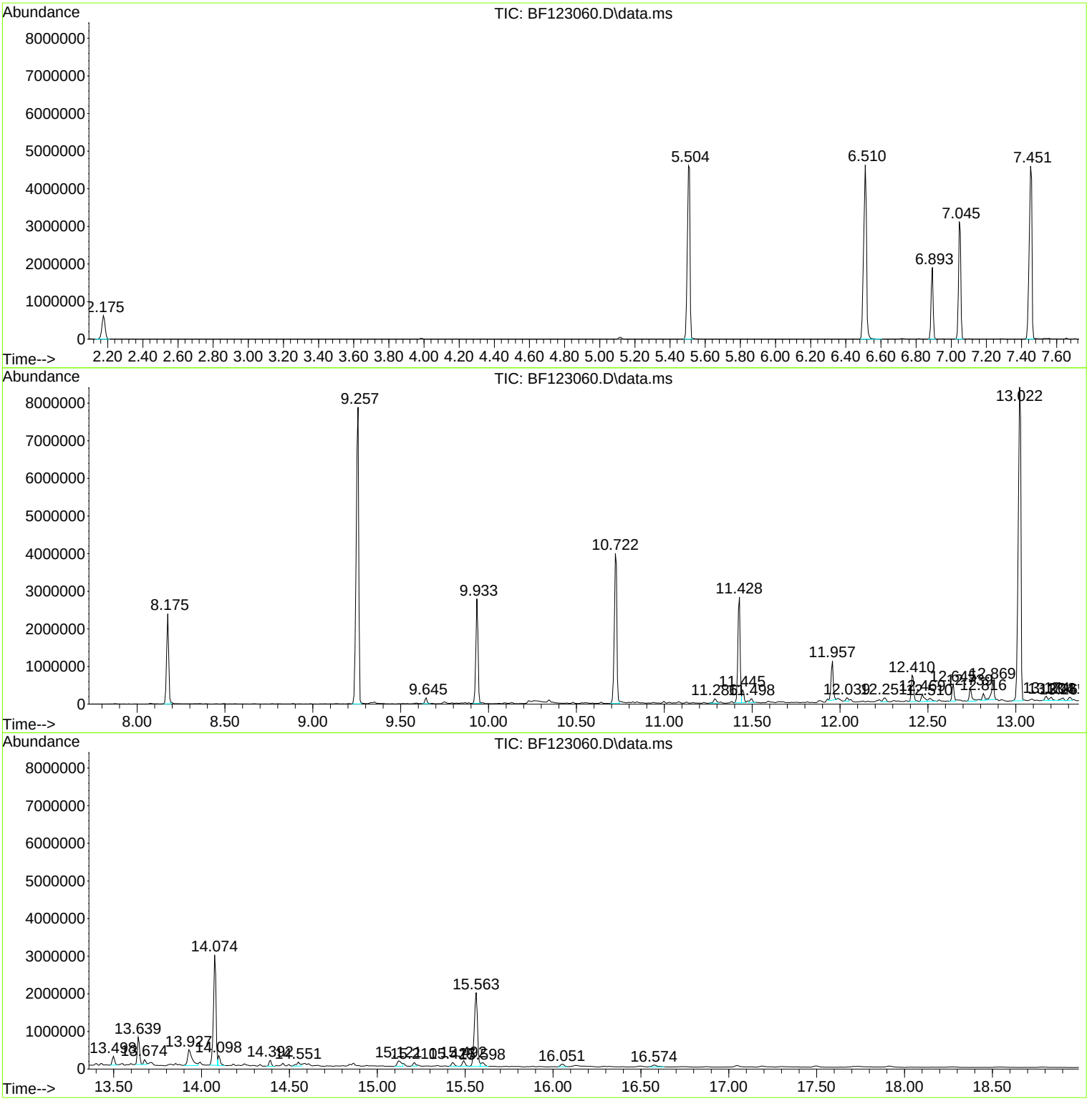
ClientSampleId :
0014-048-COMP-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123060.D
Acq On : 28 Jan 2021 15:30
Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0014-048-COMP-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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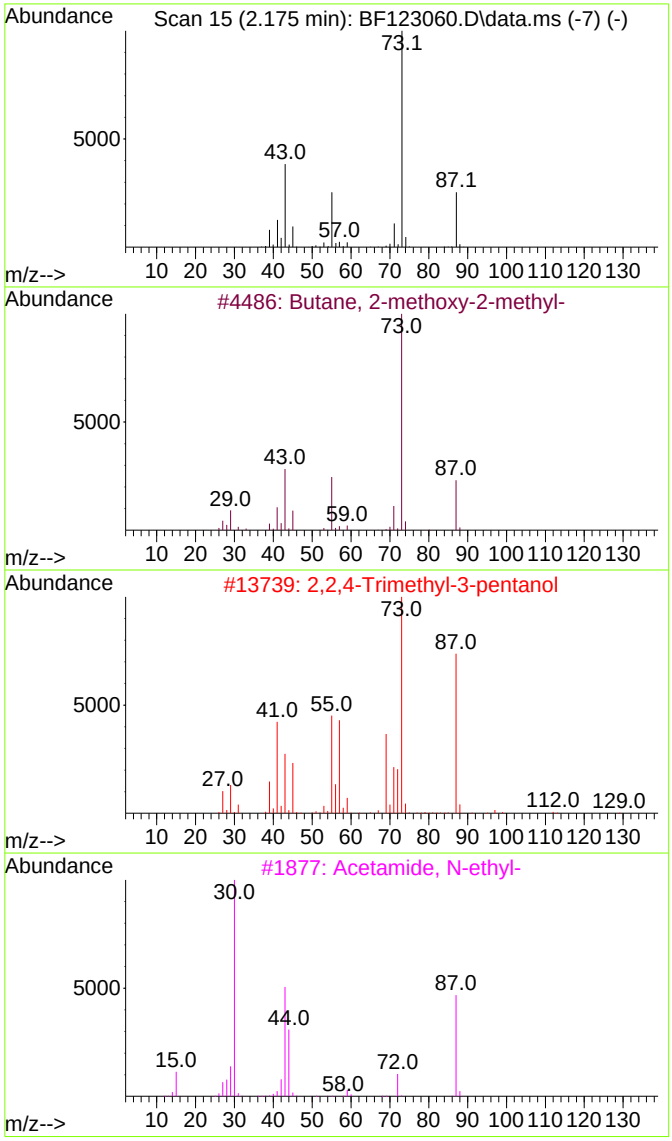
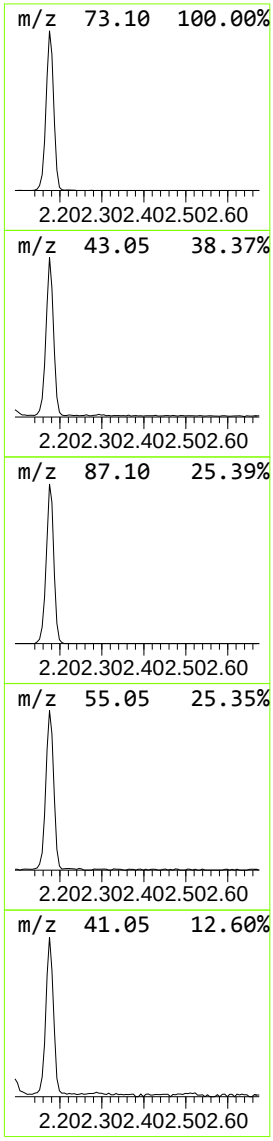
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	10.38 ng	790365	1,4-Dichlorobenzene-d4	6.893

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123060.D
Acq On : 28 Jan 2021 15:30
Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0014-048-COMP-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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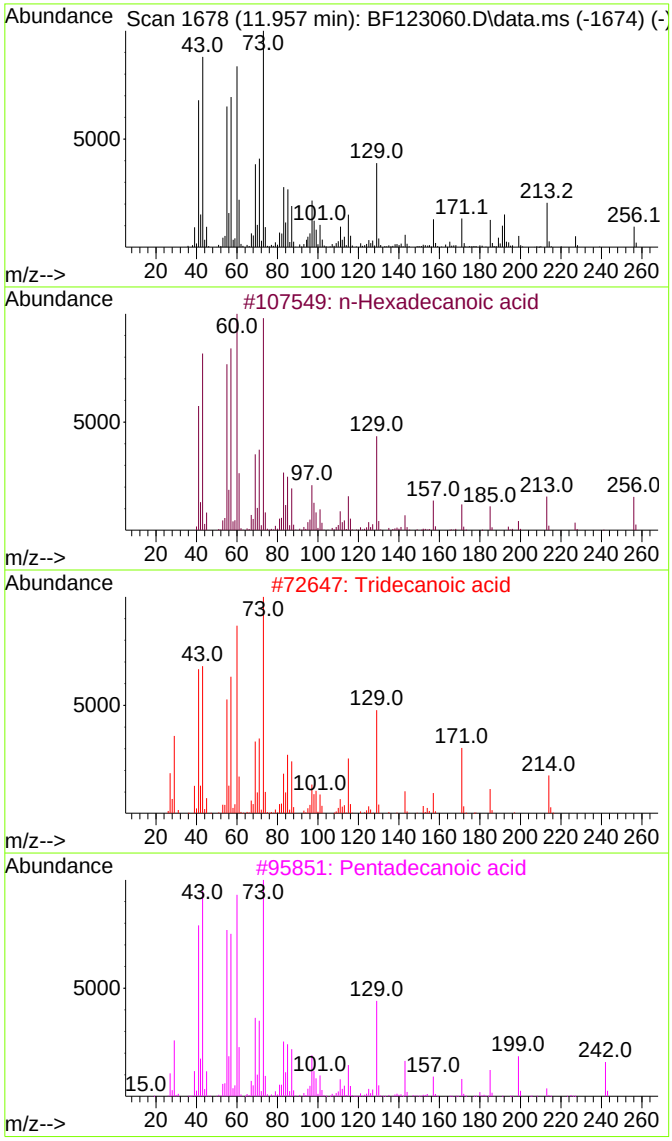
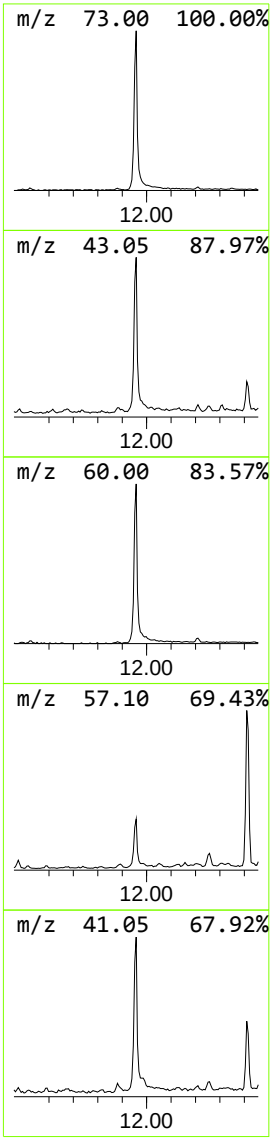
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	7.07 ng	905280	Phenanthrene-d10	11.428

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Data File : BF123060.D
Acq On : 28 Jan 2021 15:30
Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0014-048-COMP-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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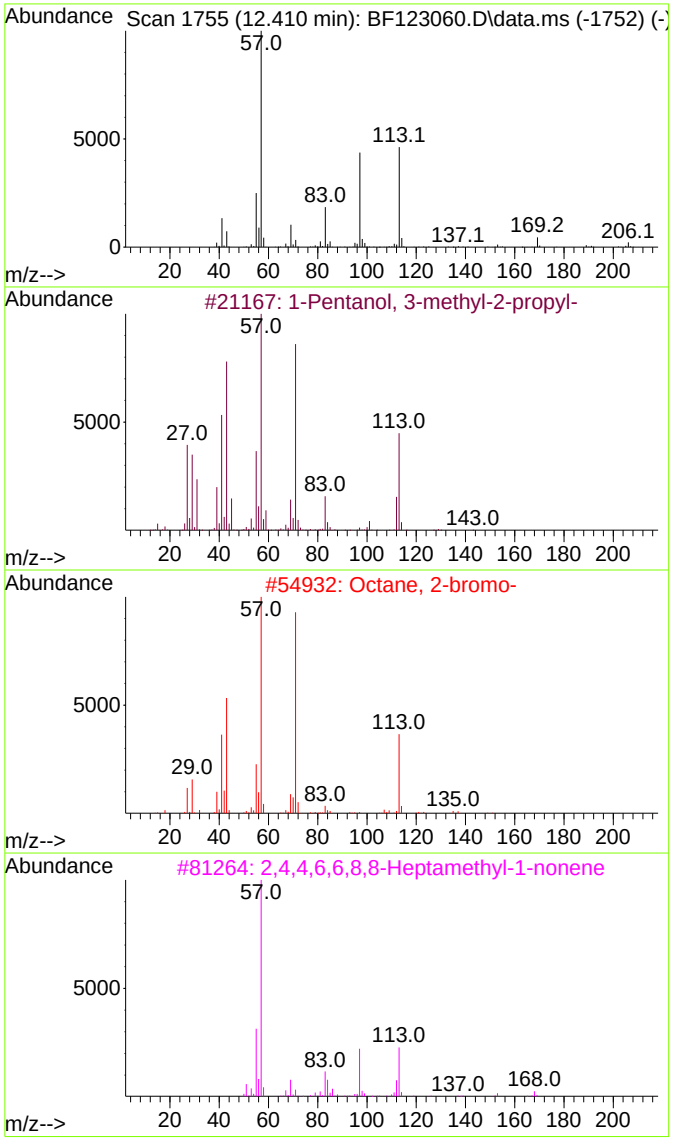
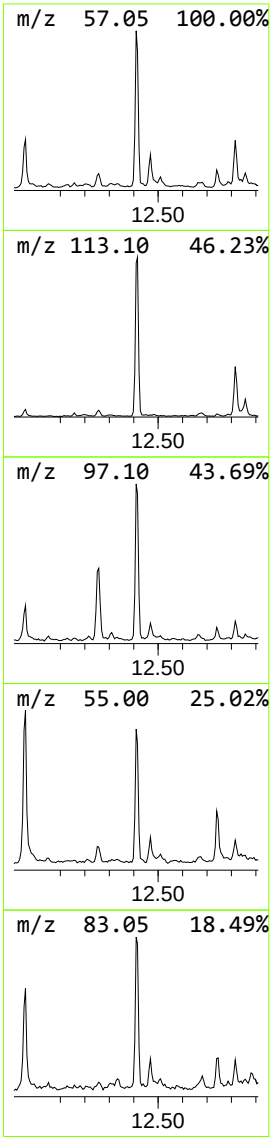
Peak Number 4 unknown12.41 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	5.06 ng	647441	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	16
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123060.D
Acq On : 28 Jan 2021 15:30
Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0014-048-COMP-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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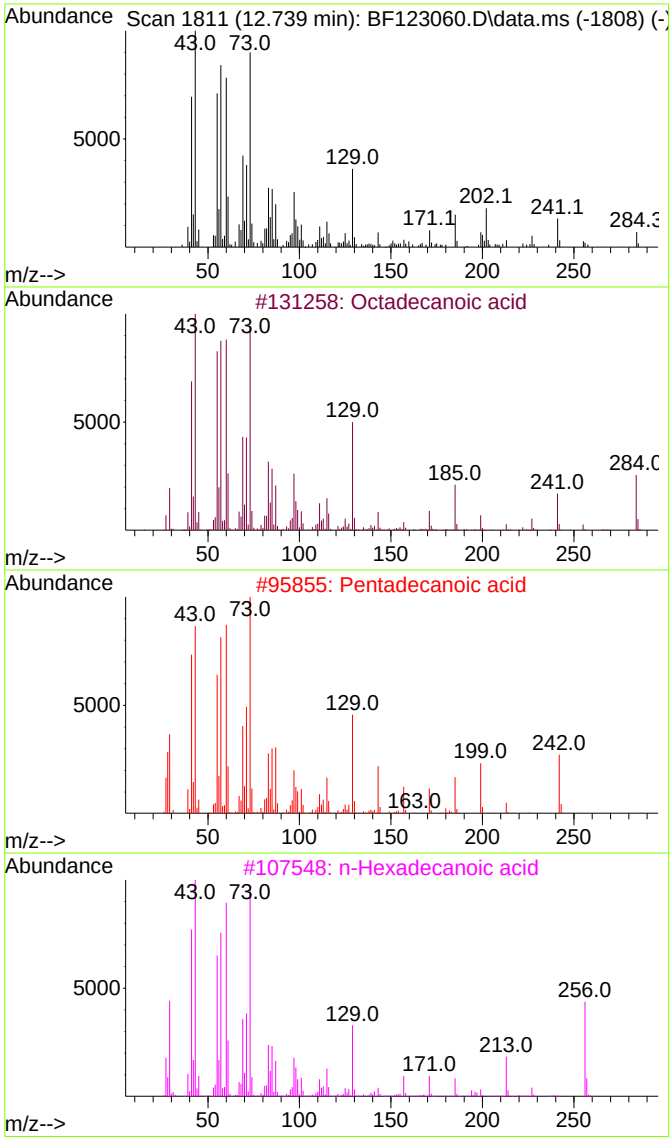
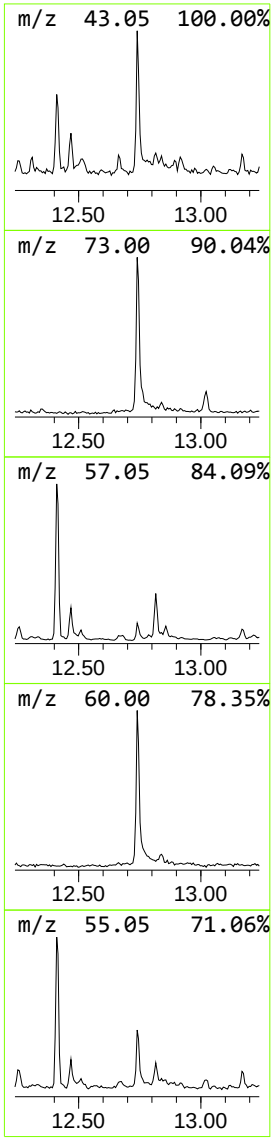
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.70 ng	345849	Phenanthrene-d10	11.428

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
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Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0014-048-COMP-G

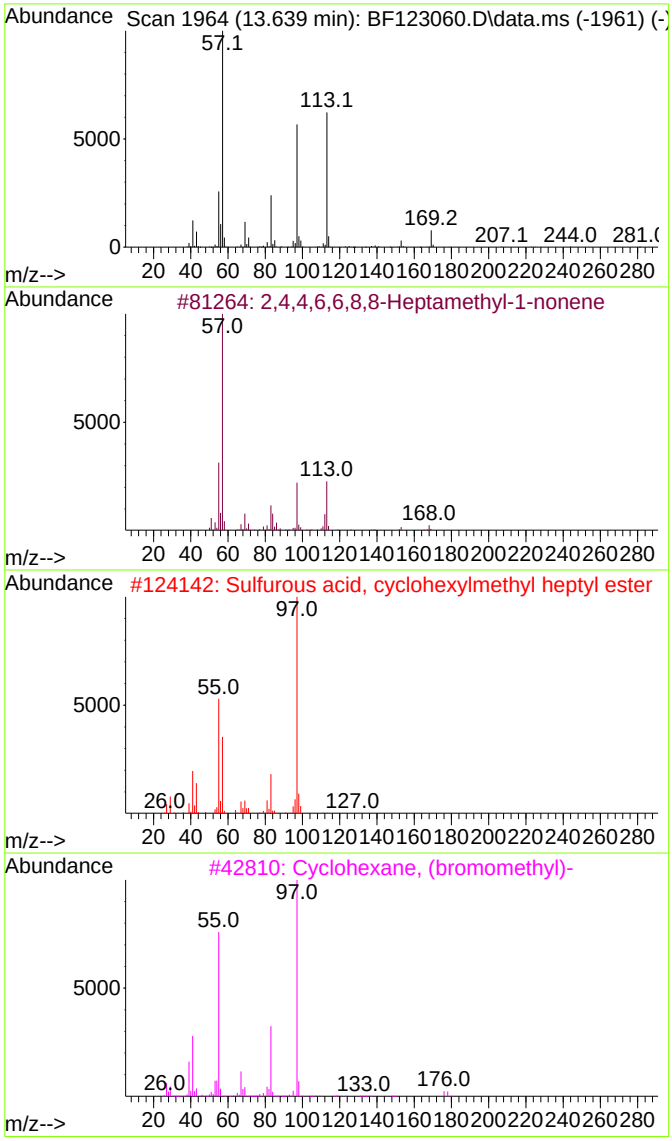
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

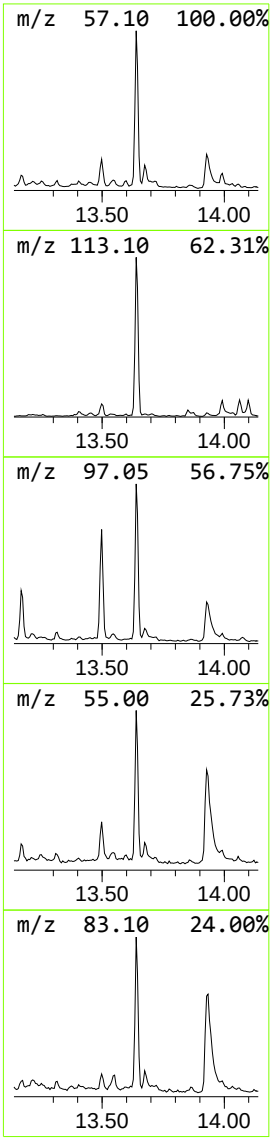
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	4.27 ng	639820	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	56
2	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	37
3	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	35
4	Phosphonofluoridic acid, ethyl-,...	196	C8H18FO2P	333416-12-9	27
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	27





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Data File : BF123060.D
Acq On : 28 Jan 2021 15:30
Operator : JU/CG
Sample : M1242-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0014-048-COMP-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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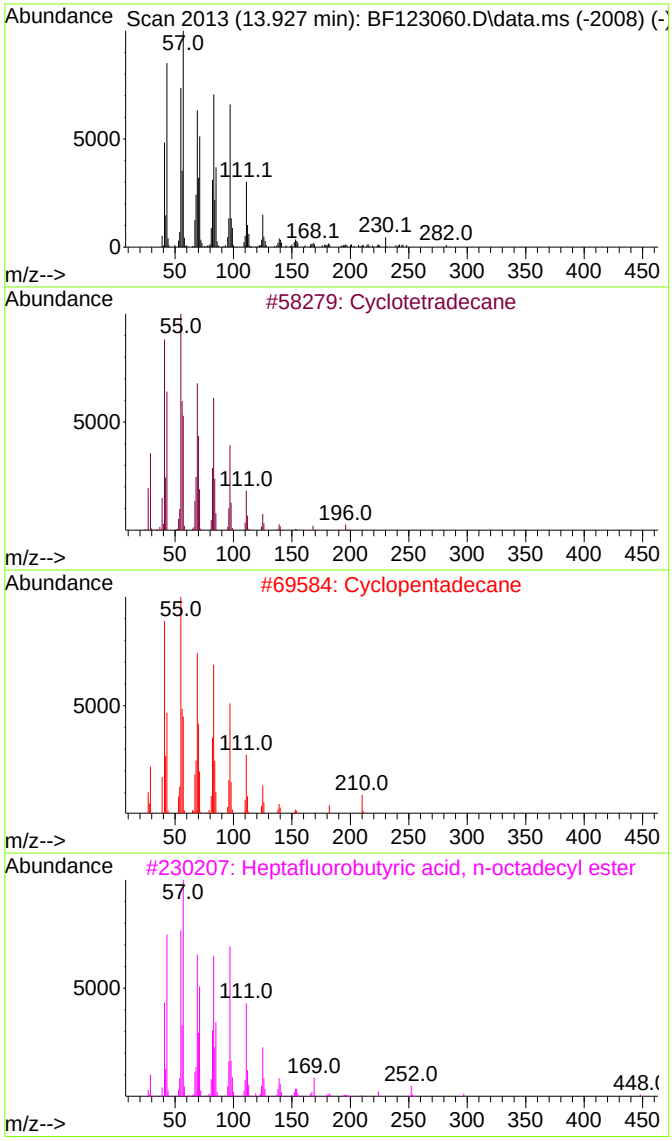
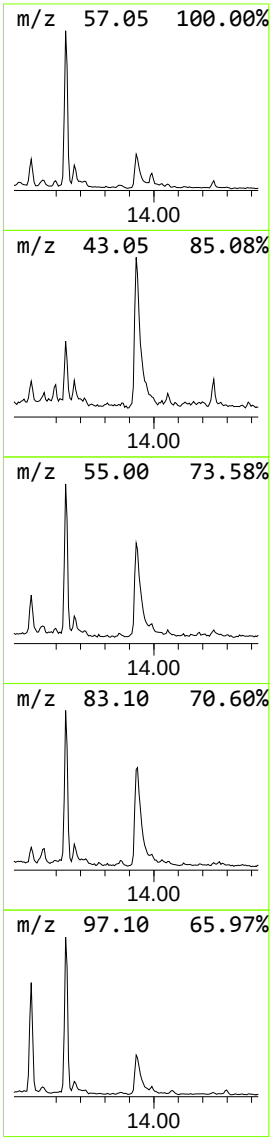
Peak Number 7 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	5.03 ng	752683	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	95
2	Cyclopentadecane	210	C15H30	000295-48-7	92
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123060.D
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Misc :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.175	10.4	ng	790365	1	6.893	1523280	20.0
n-Hexadecanoic ...	11.957	7.1	ng	905280	4	11.428	2559760	20.0
unknown12.41	12.410	5.1	ng	647441	4	11.428	2559760	20.0
Octadecanoic acid	12.739	2.7	ng	345849	4	11.428	2559760	20.0
2,4,4,6,6,8,8-H...	13.639	4.3	ng	639820	5	14.074	2993960	20.0
Cyclotetradecane	13.927	5.0	ng	752683	5	14.074	2993960	20.0