LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
Data File : BF112457.D
Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	19	rVB	131238	223828	6.36%	0.654%
2	5.057	501	505	519	rVB	104196	145752	4.14%	0.426%
3	5.475	572	576	596	rBV	2484579	2722463	77.37%	7.951%
4	6.481	743	747	765	rBV	2551589	2936309	83.45%	8.576%
5	6.610	765	769	778	rVV	3486023	3025653	85.99%	8.837%
6	6.828	803	806	812	rBV	756771	726195	20.64%	2.121%
7	6.987	829	833	837	rBV	2544383	2218840	63.06%	6.480%
8	7.392	898	902	912	rBV	1690611	1808303	51.39%	5.281%
9	8.110	1020	1024	1038	rBV	912281	967726	27.50%	2.826%
10	9.186	1202	1207	1210	rBV	3550979	3171946	90.15%	9.264%
11	9.581	1269	1274	1279	rBV	187751	168980	4.80%	0.494%
12	9.869	1318	1323	1331	rVB	1239871	1141863	32.45%	3.335%
13	10.663	1453	1458	1465	rBV	2580989	2422043	68.84%	7.074%
14	11.357	1572	1576	1583	rBV	1343120	1237307	35.16%	3.614%
15	11.798	1648	1651	1657	rBV3	38847	53761	1.53%	0.157%
16	11.880	1659	1665	1673	rBV2	442015	558760	15.88%	1.632%
17	12.092	1698	1701	1703	rBV2	53576	47936	1.36%	0.140%
18	12.222	1721	1723	1728	rVB3	38982	49166	1.40%	0.144%
19	12.310	1735	1738	1743	rVB3	75855	81544	2.32%	0.238%
20	12.580	1781	1784	1786	rVB2	53590	48416	1.38%	0.141%
21	12.663	1793	1798	1803	rBV	247598	350465	9.96%	1.024%
22	12.833	1825	1827	1830	rBV	125259	99450	2.83%	0.290%
23	12.939	1841	1845	1849	rBV	3711307	3518612	100.00%	10.276%
24	13.169	1881	1884	1886	rBV	113290	105147	2.99%	0.307%
25	13.321	1906	1910	1913	rBV3	53143	91055	2.59%	0.266%
26	13.457	1931	1933	1937	rBV	89113	77819	2.21%	0.227%
27	13.527	1942	1945	1950	rVB2	101535	110380	3.14%	0.322%
28	13.774	1985	1987	1990	rVB2	76265	79005	2.25%	0.231%
29	13.827	1992	1996	1999	rBV2	403157	569385	16.18%	1.663%
30	14.004	2020	2026	2029	rBV	1219340	1183794	33.64%	3.457%
31	14.145	2046	2050	2053	rBV2	216474	266204	7.57%	0.777%
32	14.286	2072	2074	2077	rBV	61095	53423	1.52%	0.156%
33	14.451	2098	2102	2107	rVB	292070	281541	8.00%	0.822%
34	14.551	2116	2119	2121	rVB	63422	57296	1.63%	0.167%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
Data File : BF112457.D
Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.598	2124	2127	2130	rBV2	88226	81656	2.32%	0.238%
36	14.751	2150	2153	2157	rVB	467958	493310	14.02%	1.441%
37	15.086	2202	2210	2214	rBV2	542074	764356	21.72%	2.232%
38	15.474	2267	2276	2284	rVB3	742257	1536311	43.66%	4.487%
39	15.886	2342	2346	2351	rVB	276862	407594	11.58%	1.190%
40	16.386	2427	2431	2443	rVB2	142530	308485	8.77%	0.901%
41	16.568	2459	2462	2467	rVB6	29842	48079	1.37%	0.140%

Sum of corrected areas: 34240158

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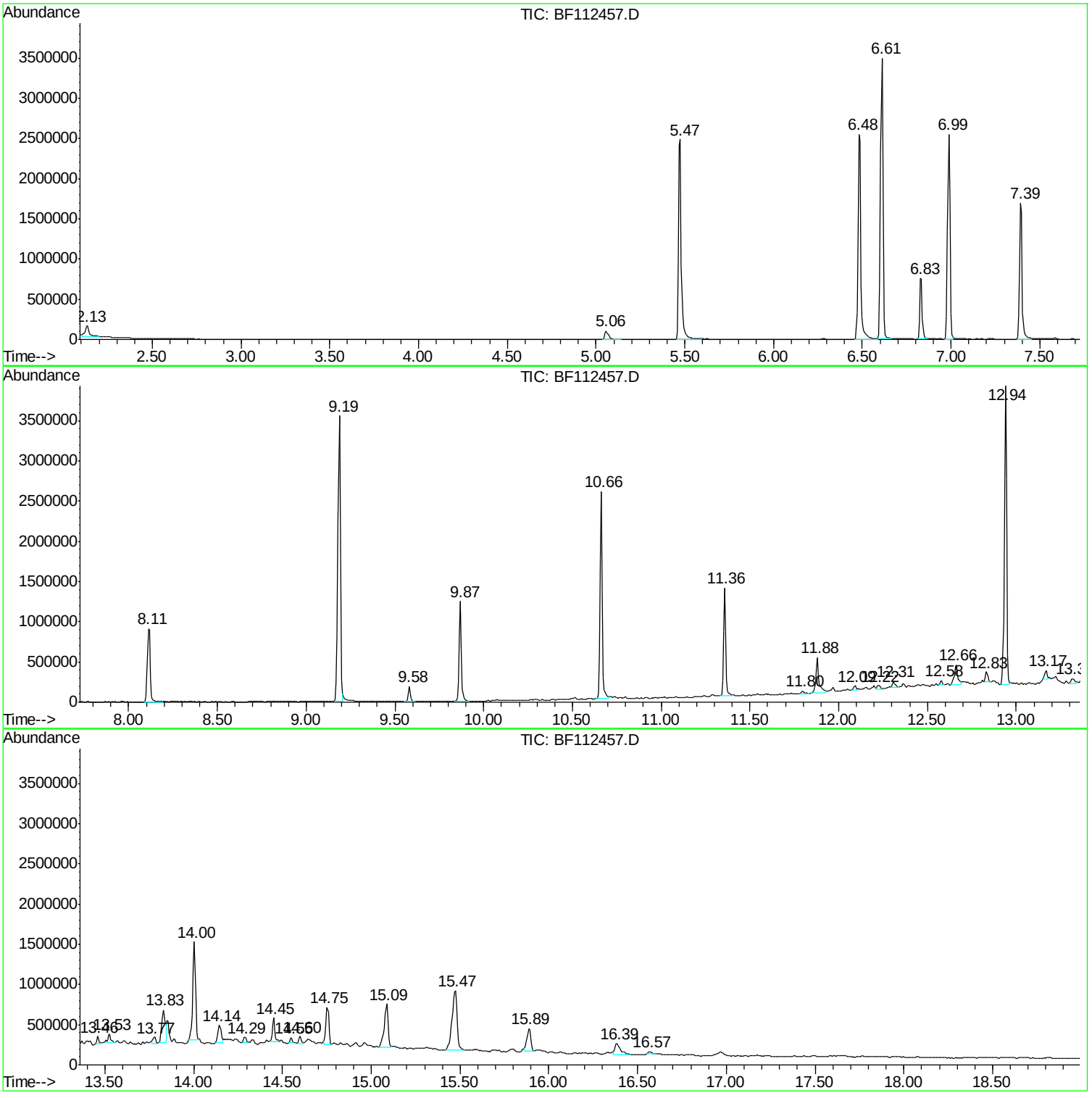
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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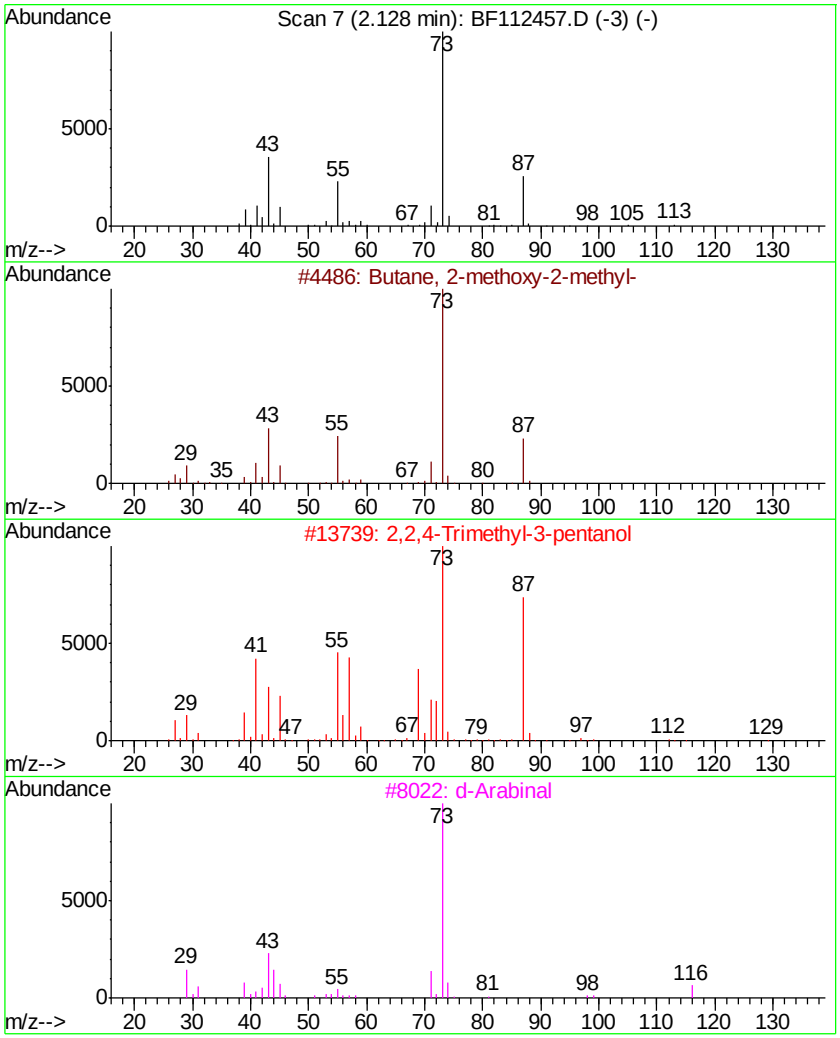
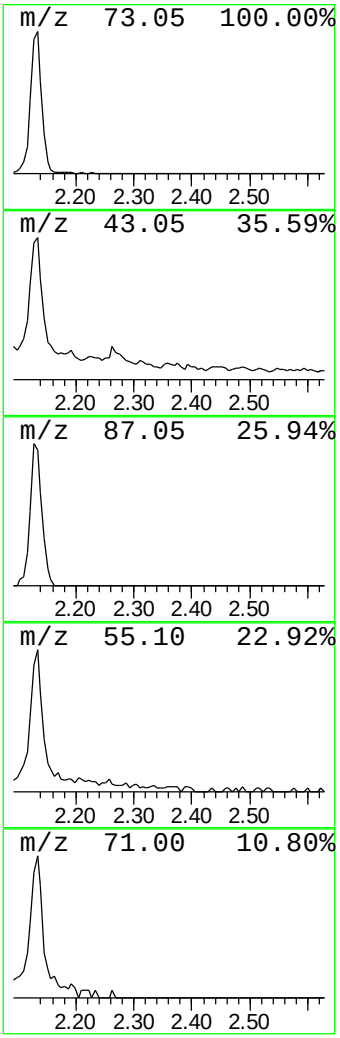
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	6.16 ng	223828	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	d-Arabinal	116	C5H8O3	000496-61-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17





Library Search Compound Report

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Data File : BF112457.D
Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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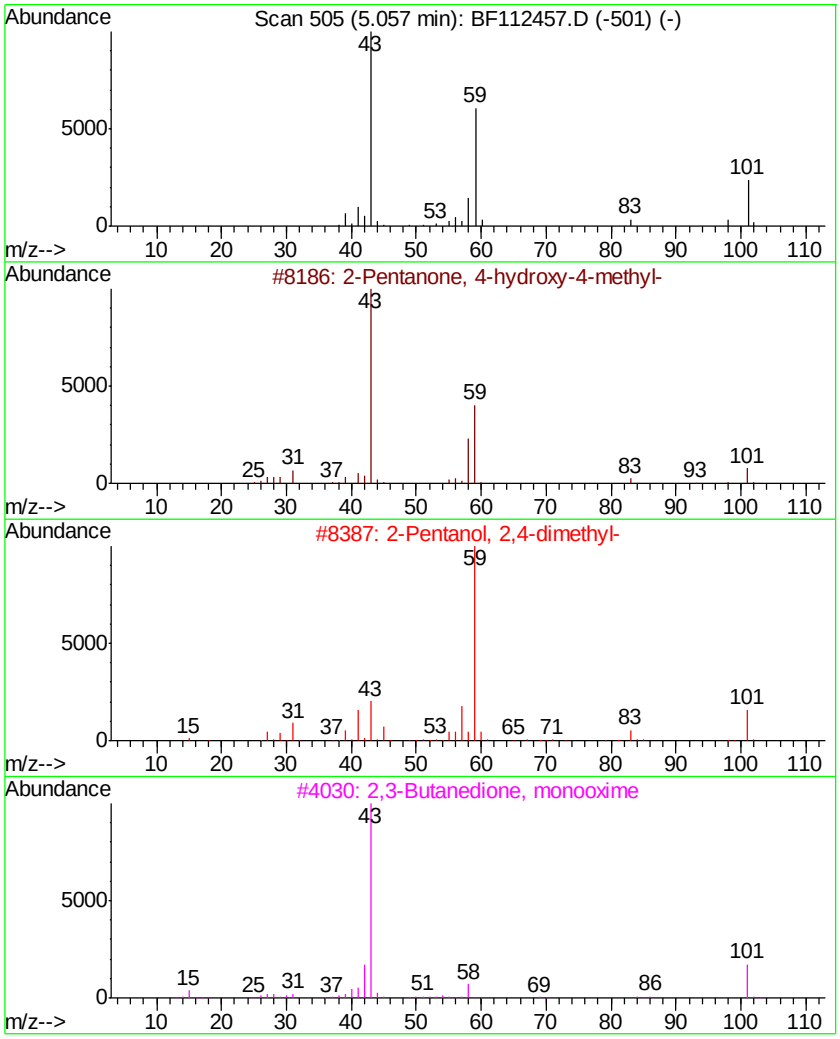
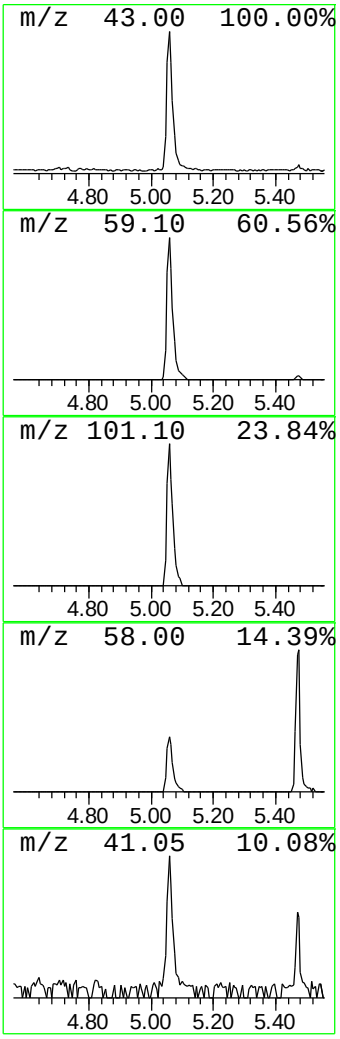
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	4.01 ng	145752	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
Data File : BF112457.D
Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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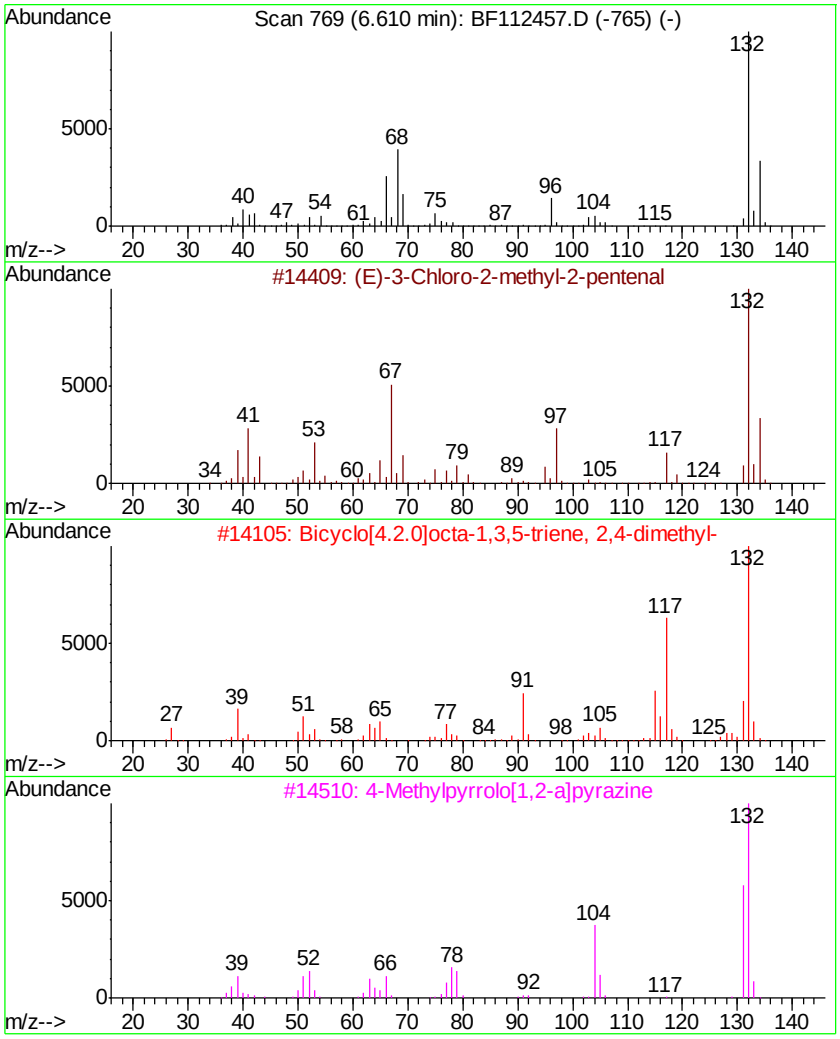
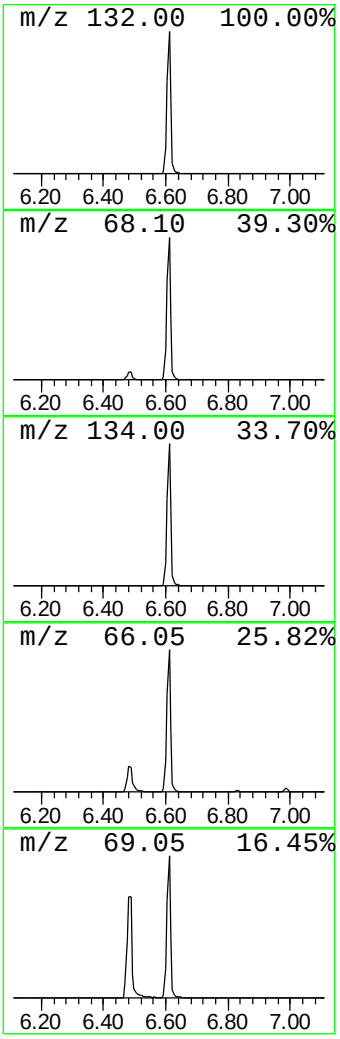
Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	83.33 ng	3025650	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
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Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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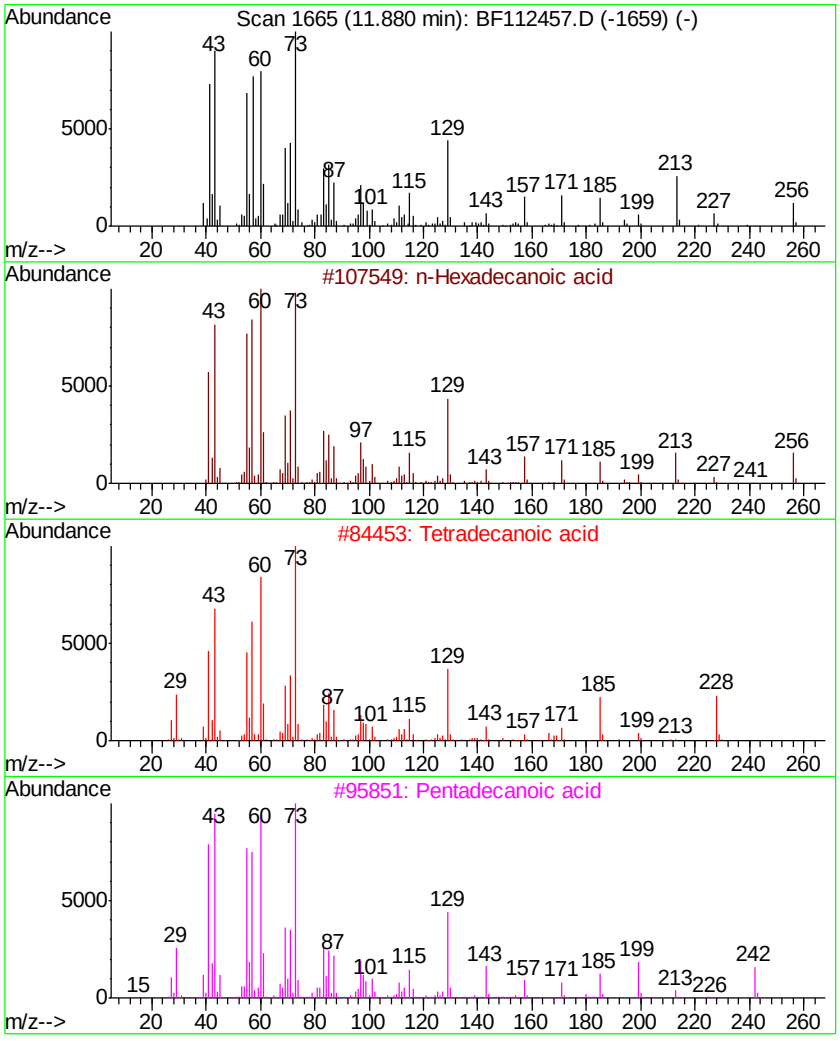
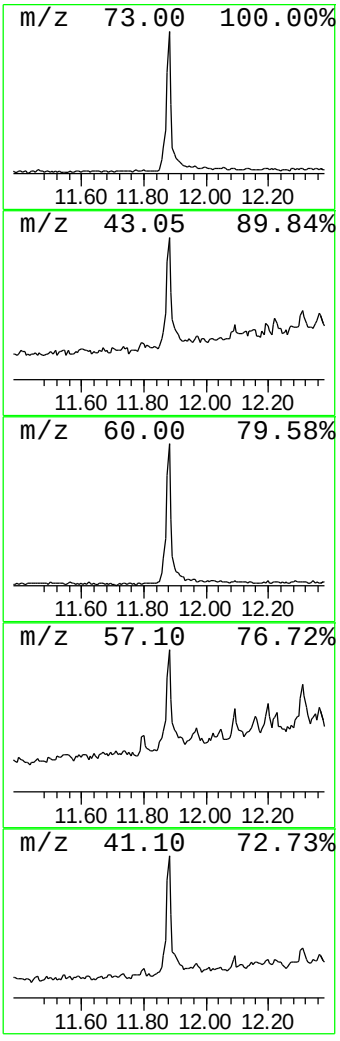
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	9.03 ng	558760	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Dodecanoic acid	200	C12H24O2	000143-07-7	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
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Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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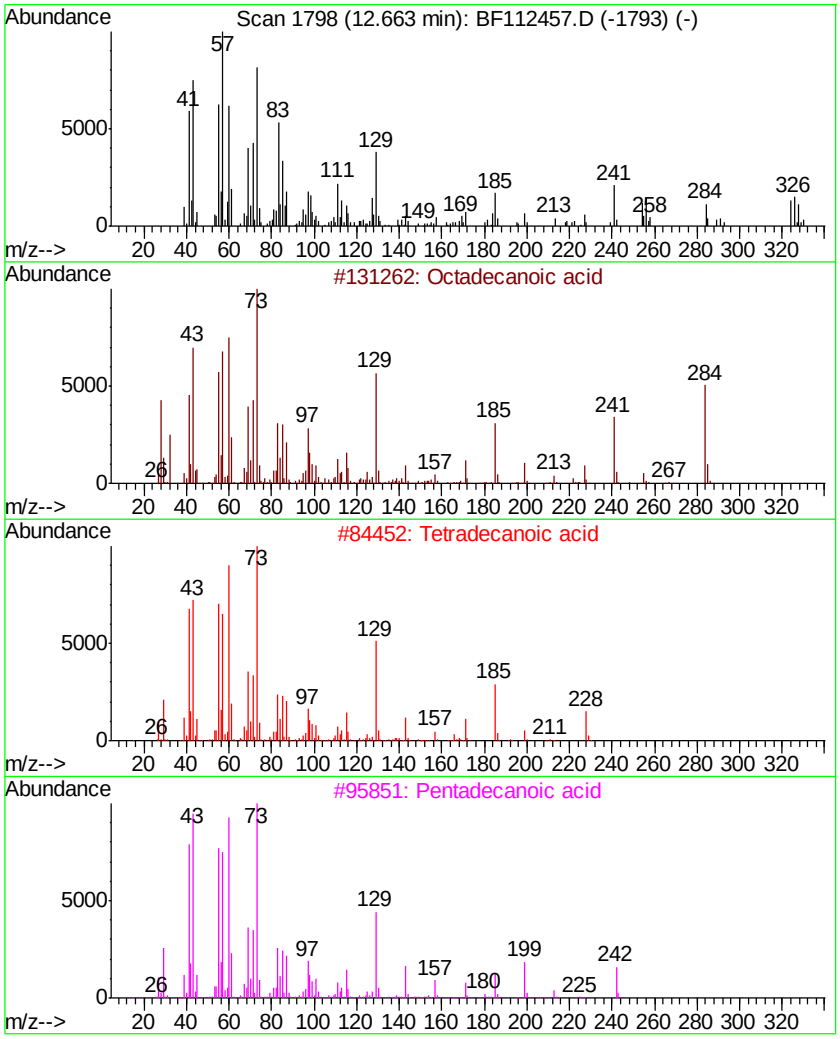
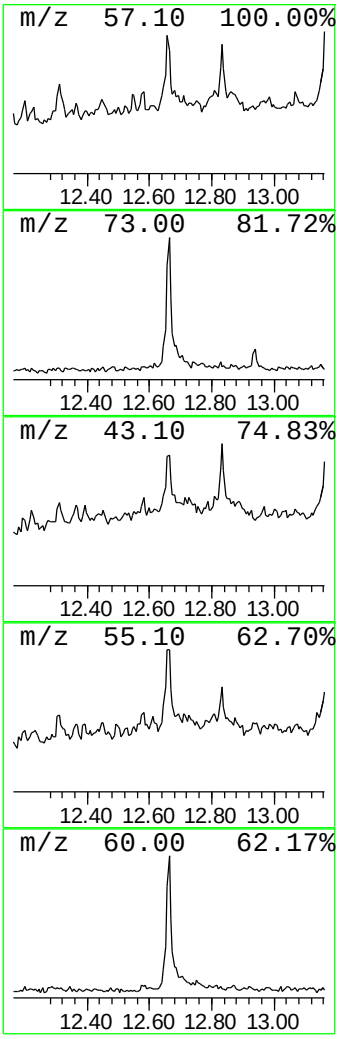
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	5.66 ng	350465	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	42
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	35





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Sample : K1422-01
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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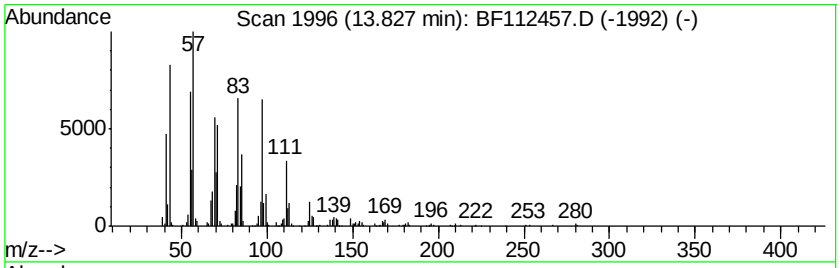
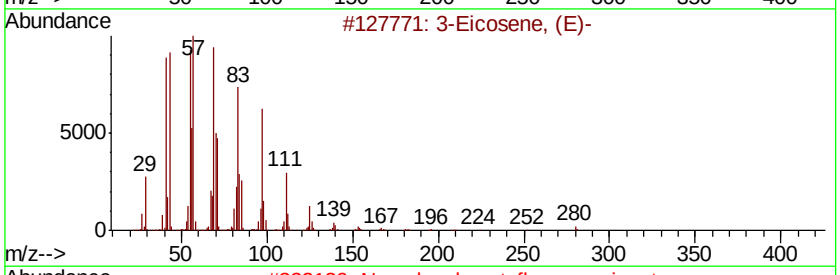
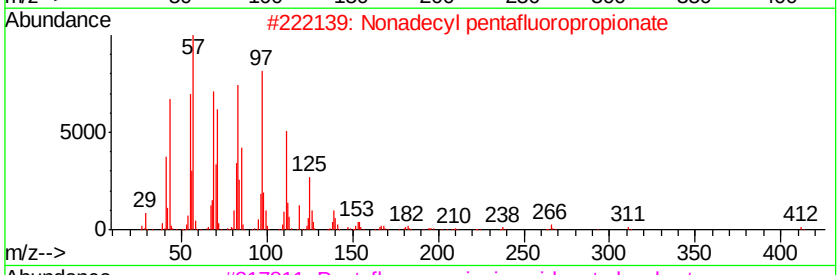
Peak Number 7 3-Eicosene, (E)- Concentration Rank 4

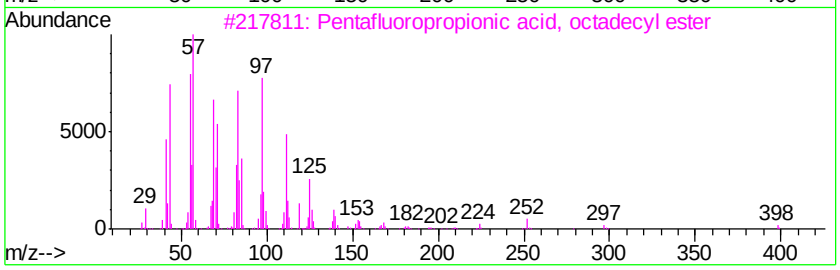
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	9.62 ng	569385	Chrysene-d12	14.00

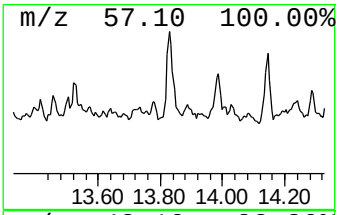
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	76

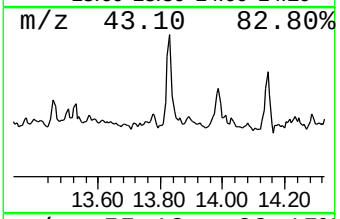


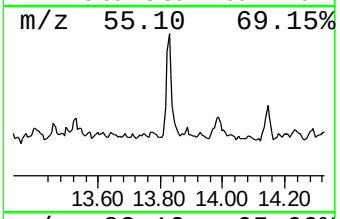


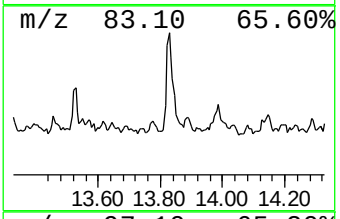


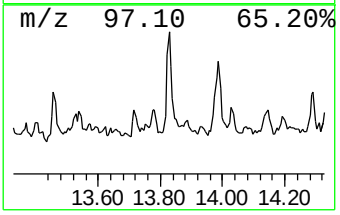












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Data File : BF112457.D
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Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

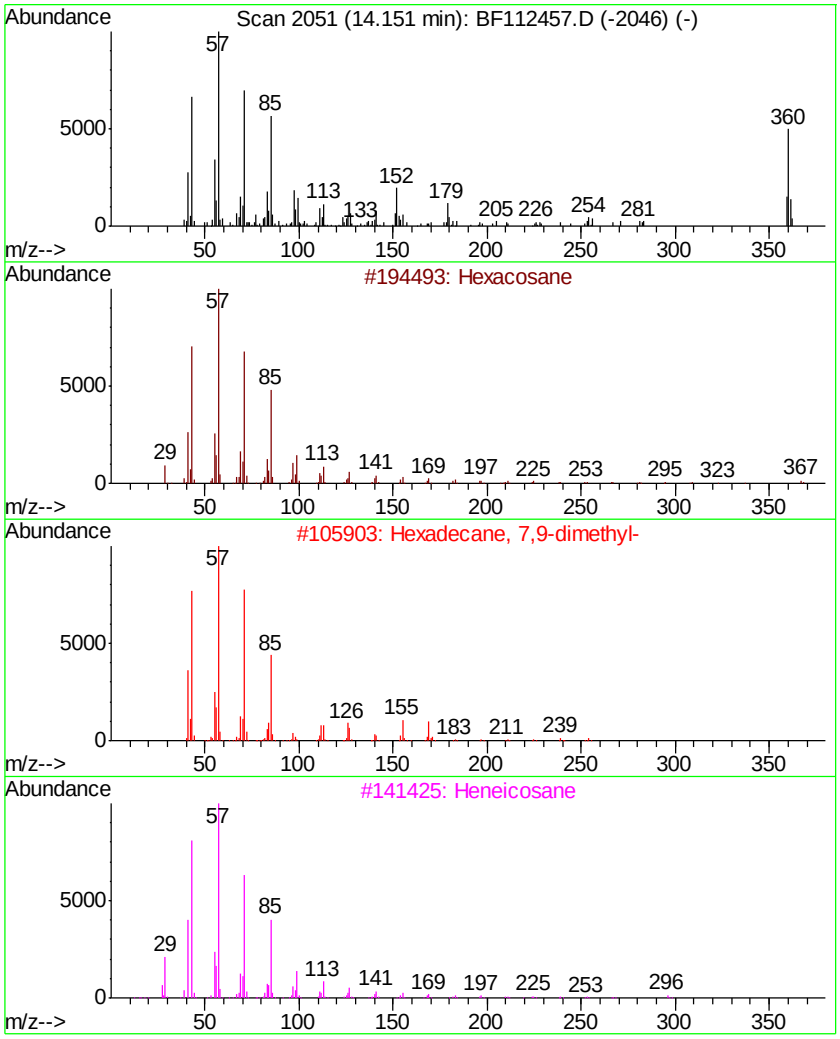
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

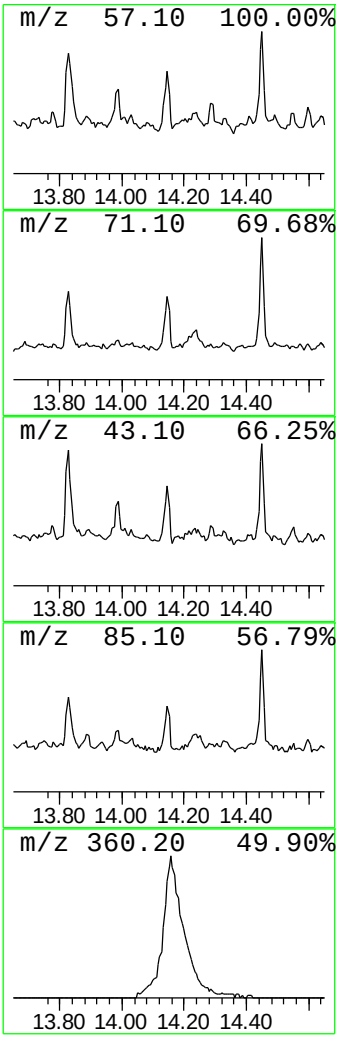
****

Peak Number 8 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	4.50 ng	266204	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	70
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	70
3	Heneicosane	296	C21H44	000629-94-7	64
4	Heptacosane	380	C27H56	000593-49-7	64
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64





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Data File : BF112457.D
Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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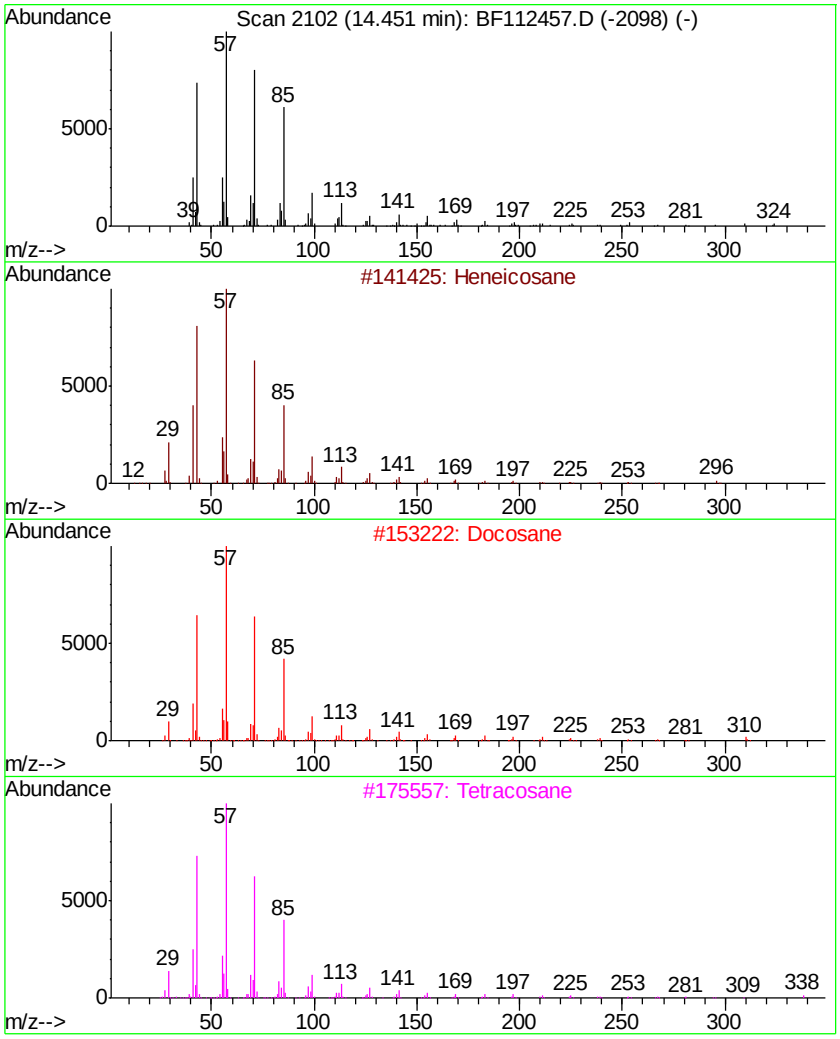
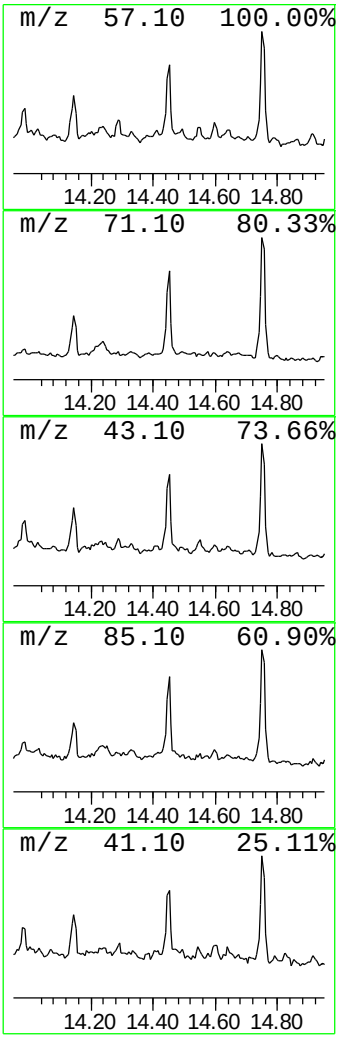
Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	4.76 ng	281541	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Docosane	310	C22H46	000629-97-0	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptadecane	240	C17H36	000629-78-7	90





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Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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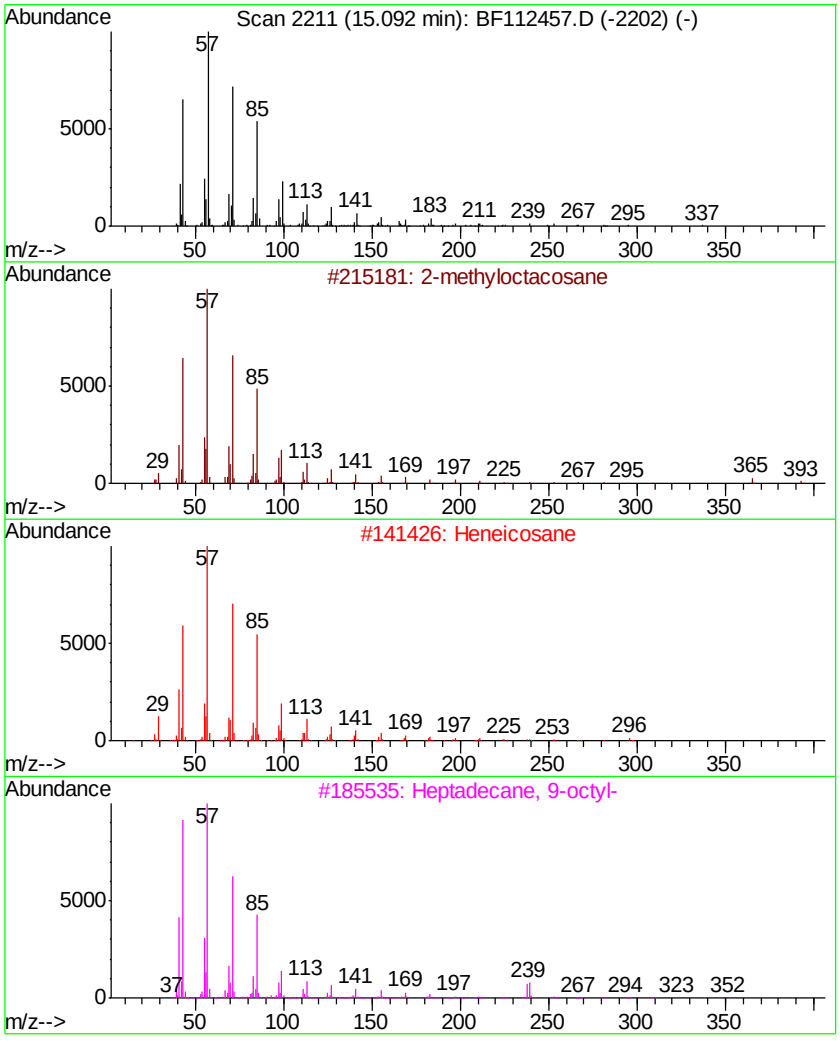
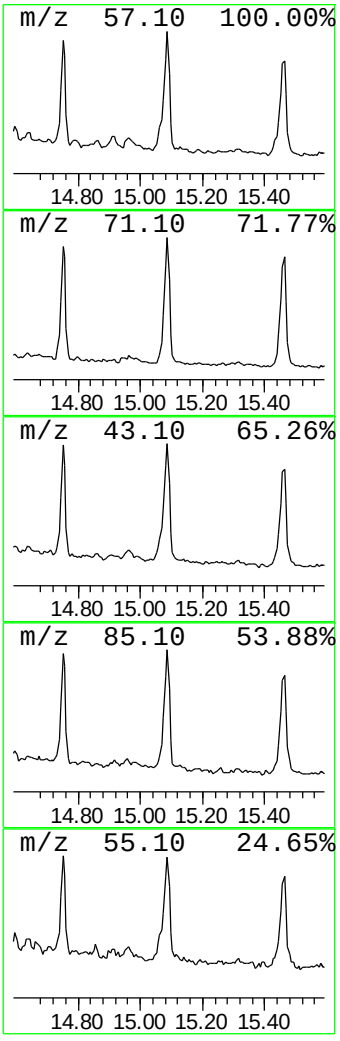
Peak Number 11 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	9.95 ng	764356	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
Data File : BF112457.D
Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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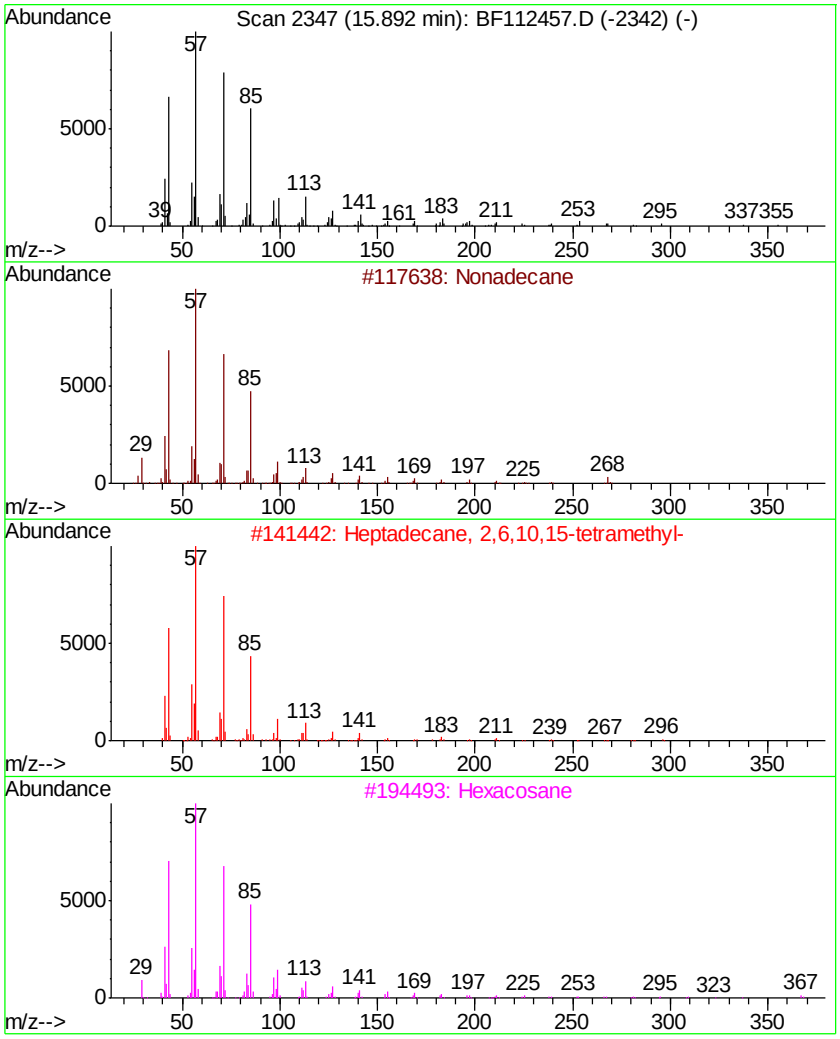
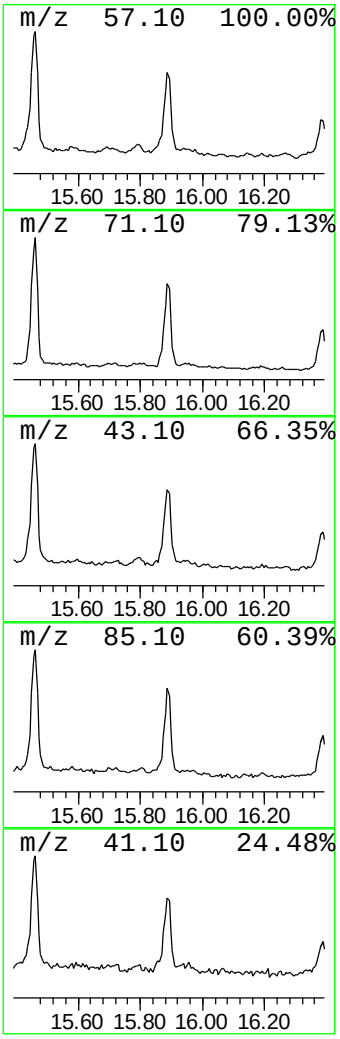
Peak Number 12 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	5.31 ng	407594	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Hexadecane	226	C16H34	000544-76-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020819\
Data File : BF112457.D
Acq On : 8 Feb 2019 14:10
Operator : JU/SJ
Sample : K1422-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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-methoxy...	2.13	6.2	ng	223828	1	6.83	726195	20.0
2-Pentanone, 4-hy...	5.06	4.0	ng	145752	1	6.83	726195	20.0
unknown6.61	6.61	83.3	ng	3025650	1	6.83	726195	20.0
n-Hexadecanoic acid	11.88	9.0	ng	558760	4	11.36	1237310	20.0
Octadecanoic acid	12.66	5.7	ng	350465	4	11.36	1237310	20.0
3-Eicosene, (E)-	13.83	9.6	ng	569385	5	14.00	1183790	20.0
Hexacosane	14.15	4.5	ng	266204	5	14.00	1183790	20.0
Heneicosane	14.45	4.8	ng	281541	5	14.00	1183790	20.0
2-methyloctacosane	15.09	9.9	ng	764356	6	15.47	1536310	20.0
Nonadecane	15.89	5.3	ng	407594	6	15.47	1536310	20.0