LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

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-BF122419.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	5.063	501	506	518	rVB	210981	276916	13.41%	1.280%
2	5.475	572	576	599	rBV	1675246	1629708	78.95%	7.531%
3	6.492	744	749	768	rBV	1578484	1691269	81.93%	7.816%
4	6.622	768	771	775	rBV	1909224	1779379	86.20%	8.223%
5	6.851	807	810	819	rBV	601292	478175	23.16%	2.210%
6	7.010	833	837	848	rBV	1635909	1412050	68.40%	6.525%
7	7.416	902	906	926	rBV	1042088	1113726	53.95%	5.147%
8	8.139	1025	1029	1049	rBV	631457	655278	31.74%	3.028%
9	9.216	1208	1212	1228	rBV	2228129	2008362	97.29%	9.281%
10	9.616	1277	1280	1289	rBV	110907	116134	5.63%	0.537%
11	9.898	1325	1328	1341	rVB	772765	790665	38.30%	3.654%
12	10.698	1460	1464	1479	rBV	1571796	1628964	78.91%	7.528%
13	11.398	1579	1583	1585	rBV	777153	793549	38.44%	3.667%
14	11.416	1585	1586	1592	rVV	233613	211380	10.24%	0.977%
15	11.474	1592	1596	1600	rVB	40100	41248	2.00%	0.191%
16	11.639	1618	1624	1628	rBV4	19095	32609	1.58%	0.151%
17	11.916	1665	1671	1679	rBV3	246414	333433	16.15%	1.541%
18	12.010	1684	1687	1690	rVV2	58846	74450	3.61%	0.344%
19	12.033	1690	1691	1697	rVB	38276	32246	1.56%	0.149%
20	12.451	1758	1762	1764	rBV	38799	35451	1.72%	0.164%
21	12.616	1786	1790	1795	rBV	321527	297399	14.41%	1.374%
22	12.704	1802	1805	1812	rVB2	56875	60061	2.91%	0.278%
23	12.845	1823	1829	1836	rVB	256278	283508	13.73%	1.310%
24	12.986	1848	1853	1856	rBV	2256681	2064272	100.00%	9.539%
25	13.069	1862	1867	1872	rVB4	19176	30574	1.48%	0.141%
26	13.280	1899	1903	1905	rBV2	24139	25166	1.22%	0.116%
27	13.457	1931	1933	1938	rVB2	24712	25084	1.22%	0.116%
28	13.804	1988	1992	1994	rBV	25394	24219	1.17%	0.112%
29	13.880	2001	2005	2016	rVB3	238585	391660	18.97%	1.810%
30	14.015	2025	2028	2030	rBV	29448	26714	1.29%	0.123%
31	14.051	2030	2034	2037	rVV2	762306	795123	38.52%	3.674%
32	14.074	2037	2038	2046	rVB	121173	105483	5.11%	0.487%
33	14.198	2056	2059	2062	rBV	57343	66058	3.20%	0.305%
34	14.445	2096	2101	2103	rBV	22043	26987	1.31%	0.125%

LSC Area Percent Report

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Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.504	2108	2111	2113	rBV	98314	94650	4.59%	0.437%
36	14.663	2136	2138	2141	rBV3	39643	38308	1.86%	0.177%
37	14.810	2159	2163	2166	rVB	119210	122235	5.92%	0.565%
38	15.110	2209	2214	2218	rBV	90440	153751	7.45%	0.711%
39	15.151	2218	2221	2225	rVB2	131580	165523	8.02%	0.765%
40	15.221	2230	2233	2239	rVB4	19299	31516	1.53%	0.146%
41	15.310	2245	2248	2254	rVB7	13793	21890	1.06%	0.101%
42	15.415	2263	2266	2274	rVB	44434	54670	2.65%	0.253%
43	15.480	2274	2277	2282	rVB	62940	81275	3.94%	0.376%
44	15.545	2283	2288	2297	rBV	526474	748262	36.25%	3.458%
45	15.980	2357	2362	2368	rBV	104647	145790	7.06%	0.674%
46	16.057	2370	2375	2383	rBV8	31352	86953	4.21%	0.402%
47	16.492	2444	2449	2454	rVB	49521	82871	4.01%	0.383%
48	17.080	2536	2549	2550	rBV4	36991	104637	5.07%	0.484%
49	17.251	2569	2578	2580	rBV8	26364	64644	3.13%	0.299%
50	17.304	2583	2587	2592	rVV6	41845	91175	4.42%	0.421%
51	17.362	2592	2597	2601	rVB6	31249	64429	3.12%	0.298%
52	17.521	2619	2624	2625	rBV3	22847	28788	1.39%	0.133%
53	17.639	2638	2644	2653	rBV3	35242	100821	4.88%	0.466%

Sum of corrected areas: 21639488

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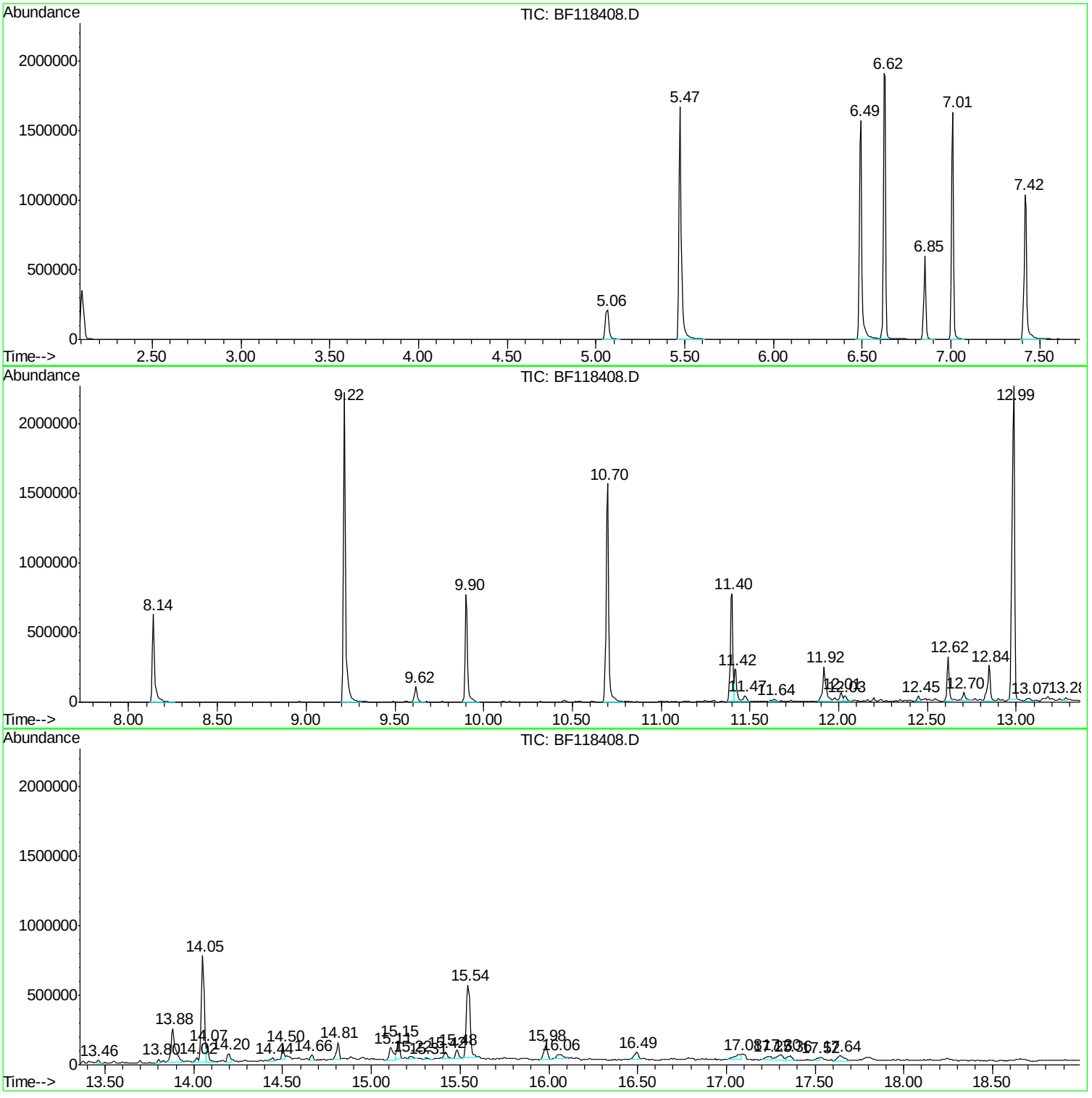
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

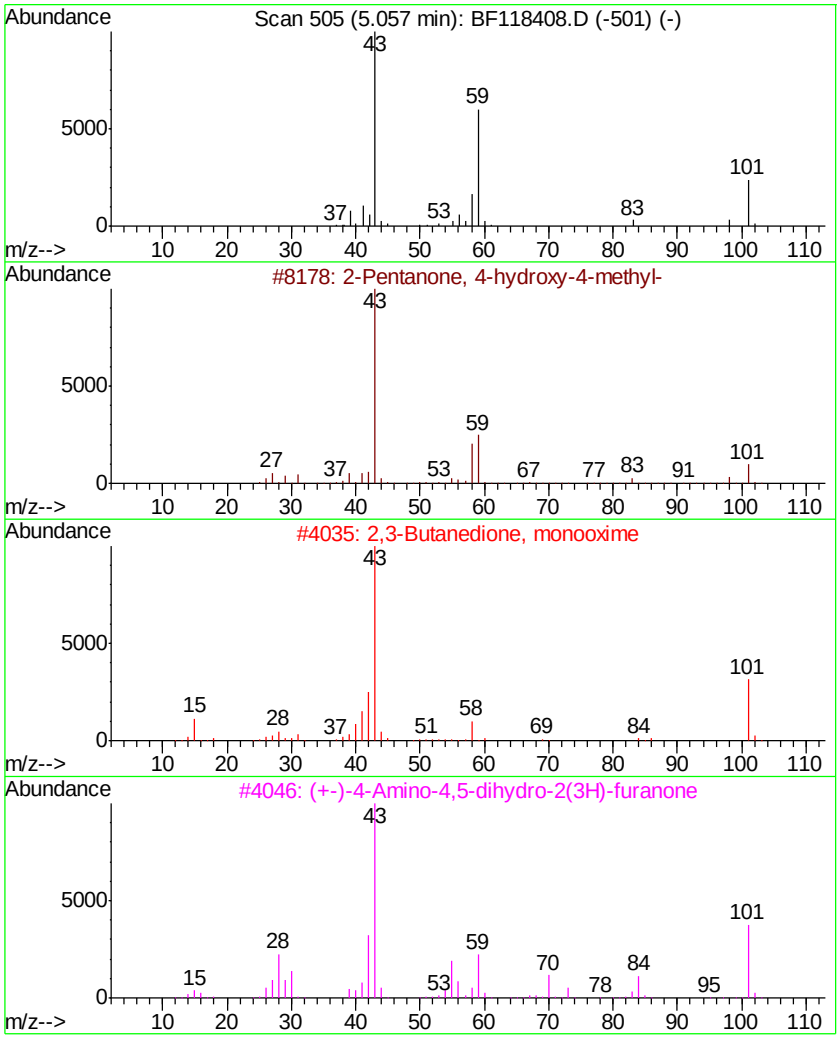
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

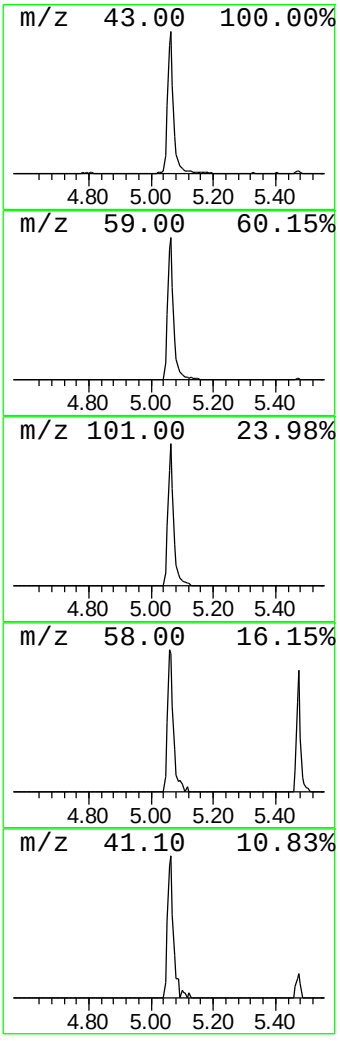
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	11.58 ng	276916	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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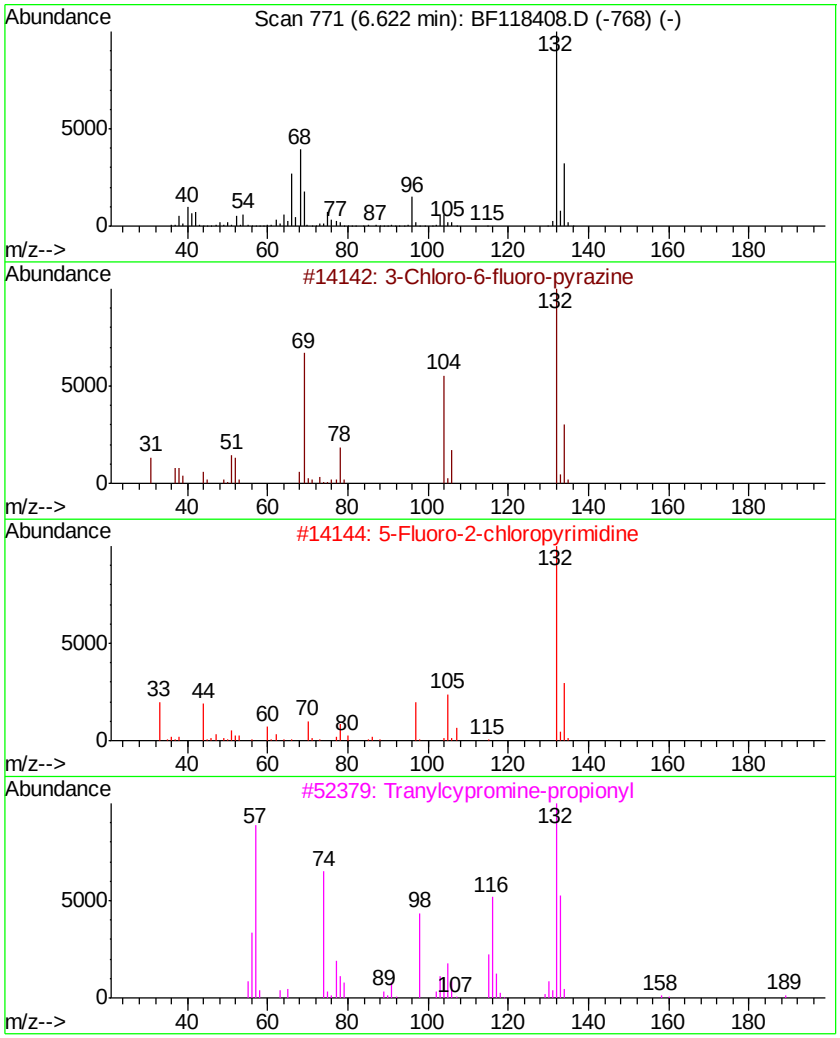
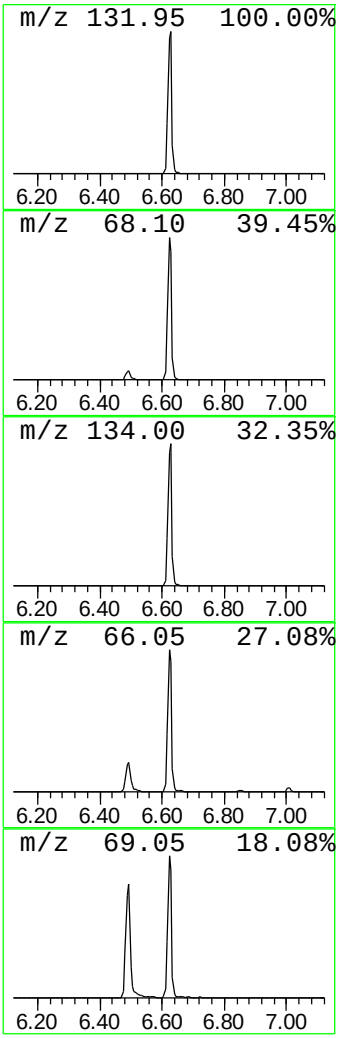
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	74.42 ng	1779380	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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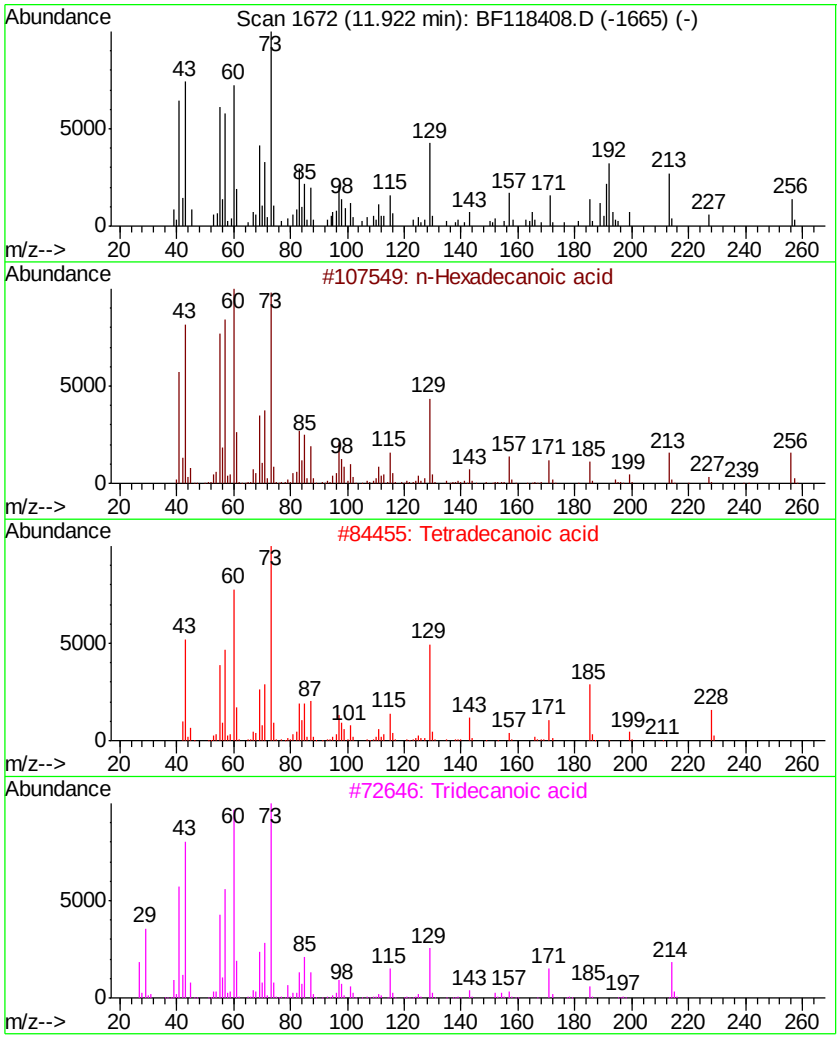
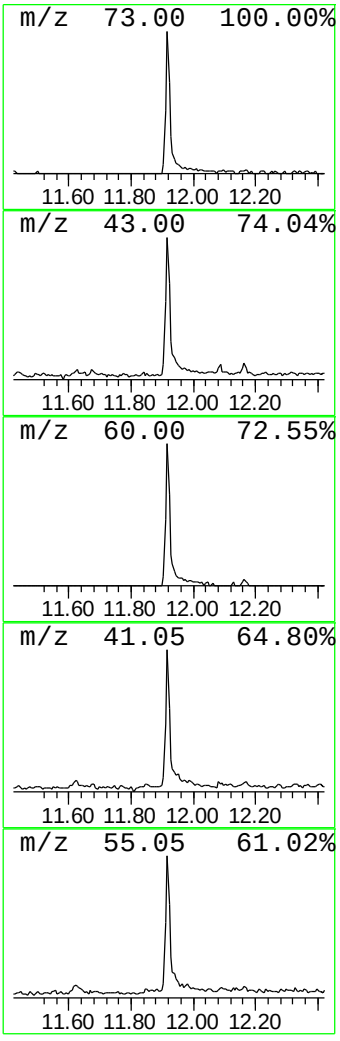
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	8.40 ng	333433	Phenanthrene-d10	11.40

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	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	41





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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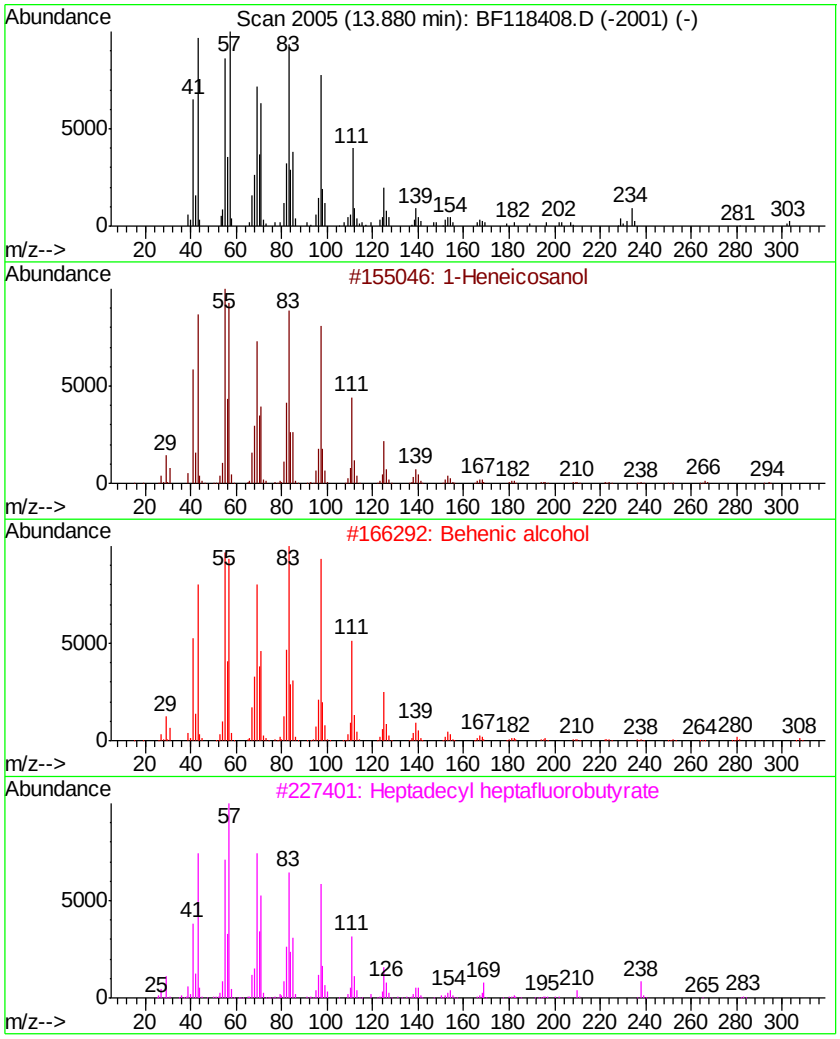
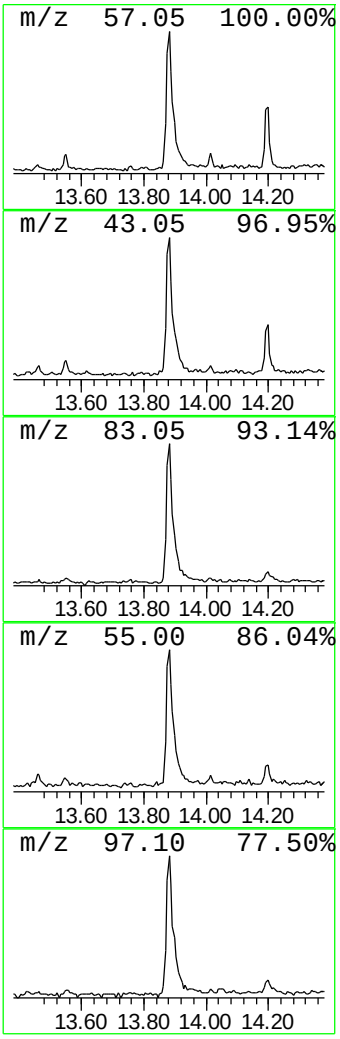
Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	9.85 ng	391660	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





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Misc :
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Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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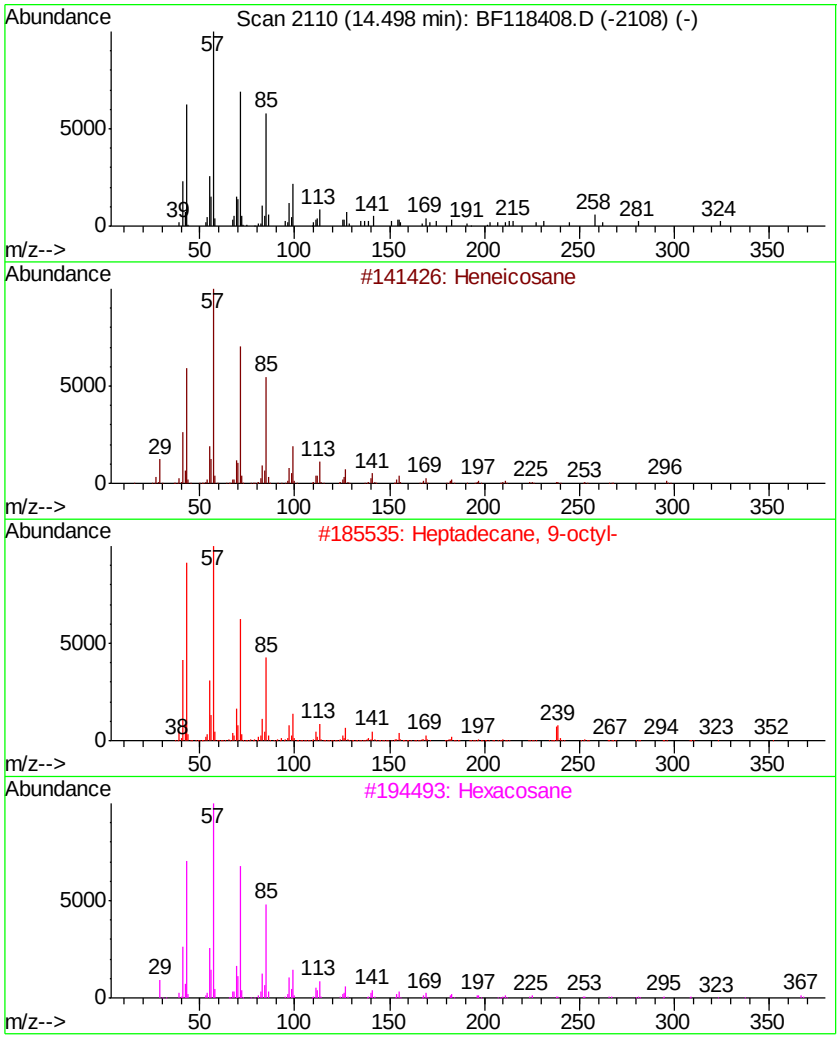
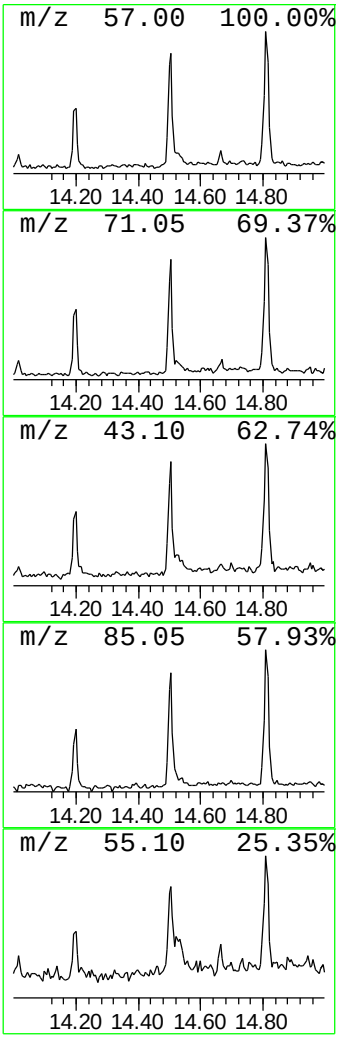
Peak Number 6 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.38 ng	94650	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Tetracosane	338	C24H50	000646-31-1	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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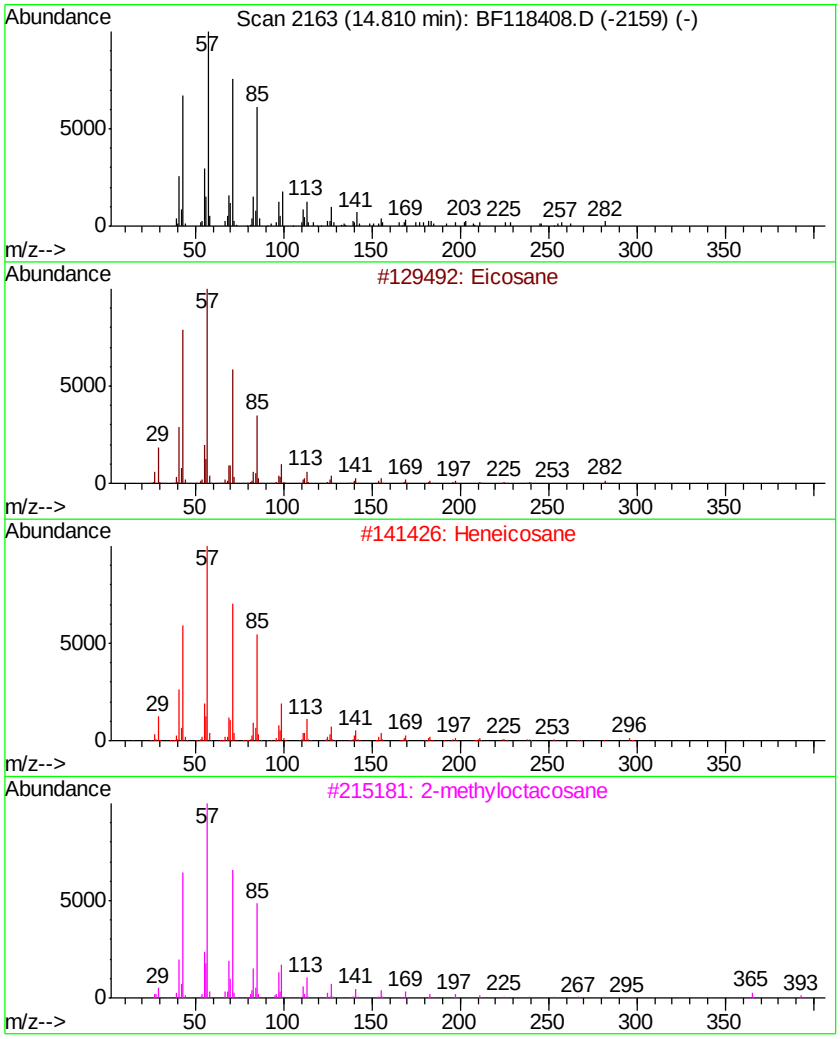
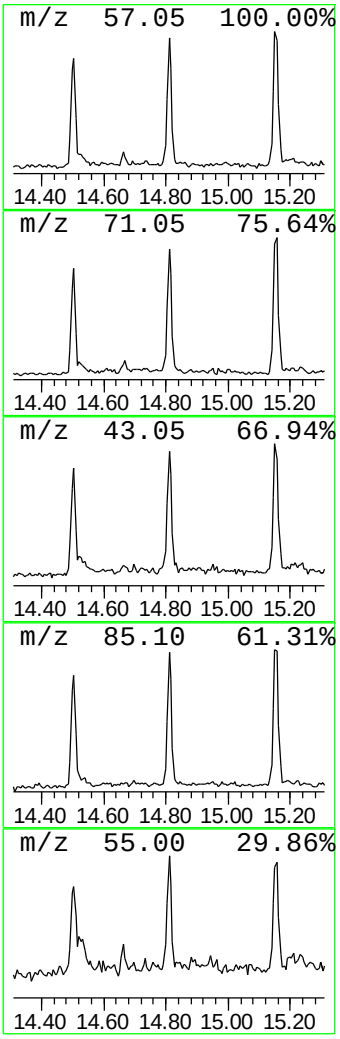
Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	3.27 ng	122235	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
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Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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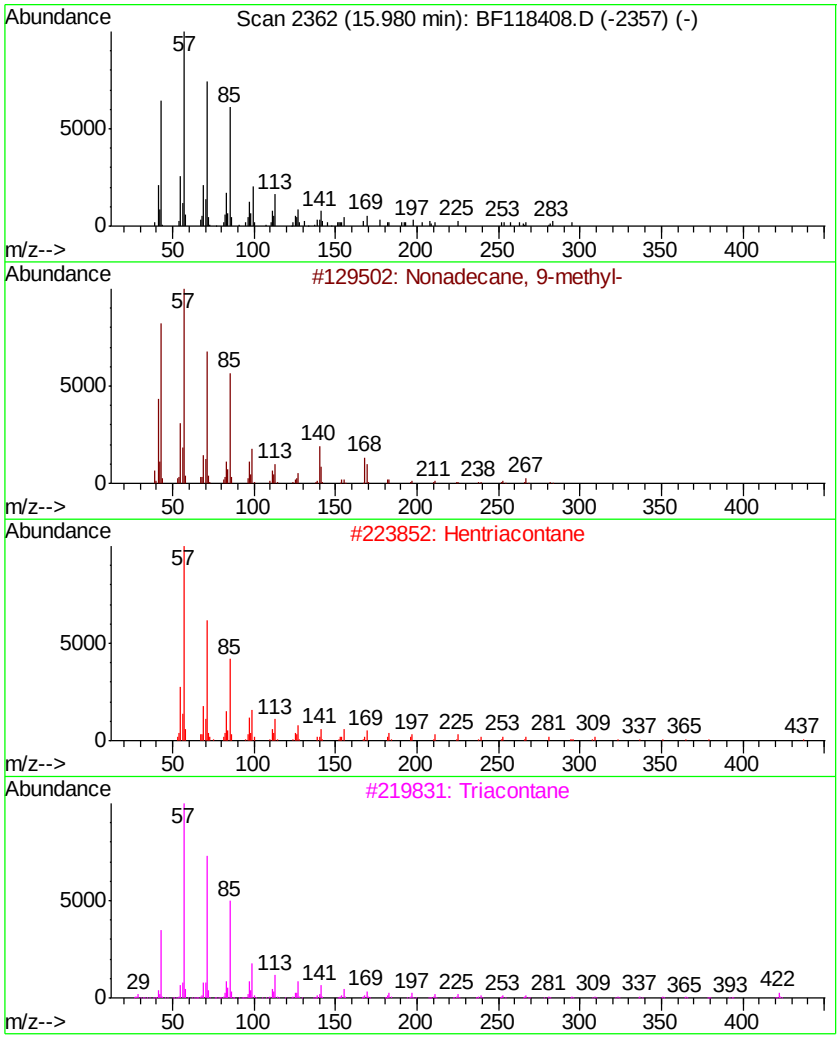
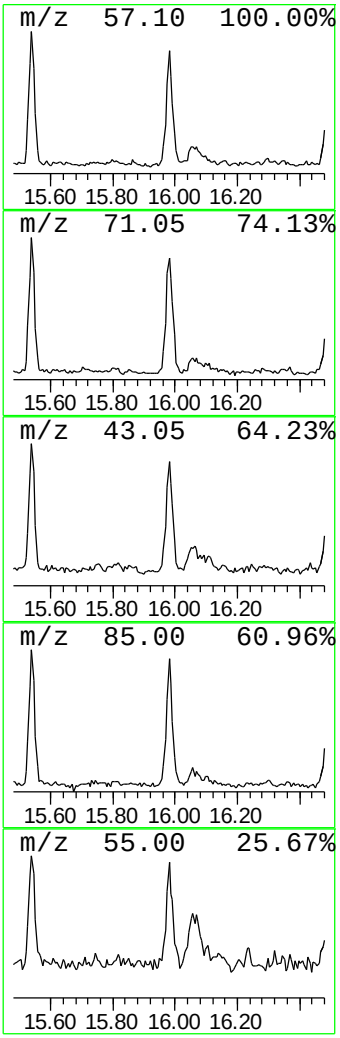
Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	3.90 ng	145790	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	95
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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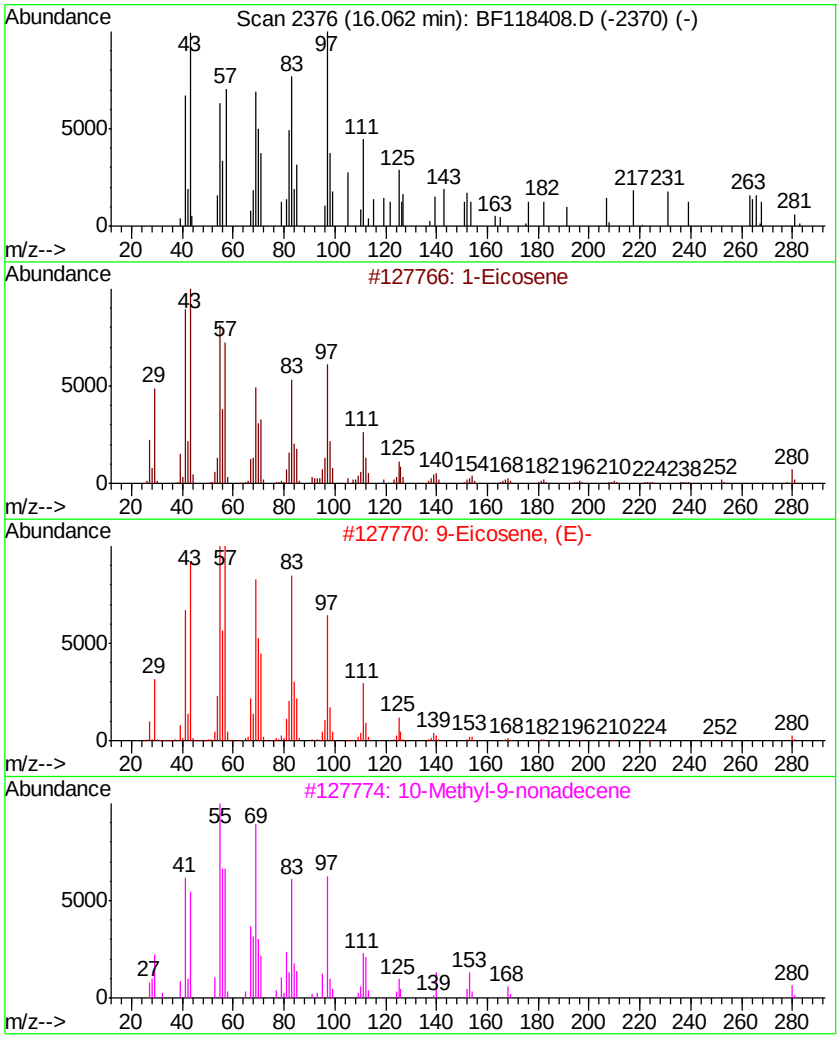
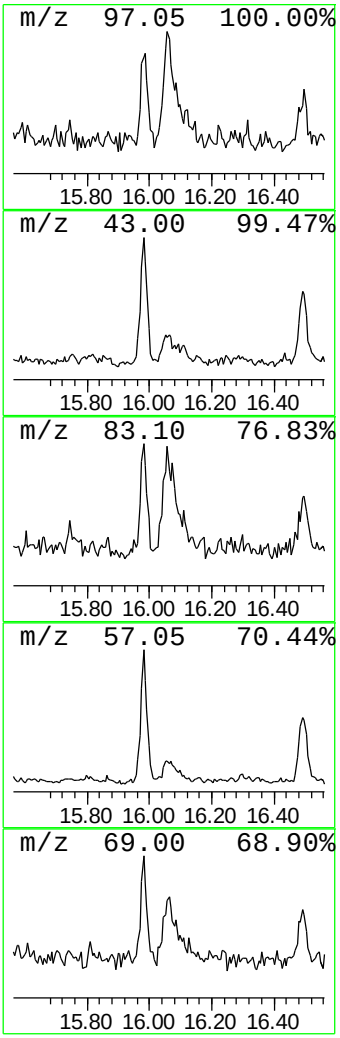
Peak Number 9 1-Eicosene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	2.32 ng	86953	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	83
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	52
3	10-Methyl-9-nonadecene	280	C20H40	1000114-07-5	52
4	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	47
5	11-Tricosene	322	C23H46	052078-56-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118408.D
Acq On : 31 Dec 2019 16:34
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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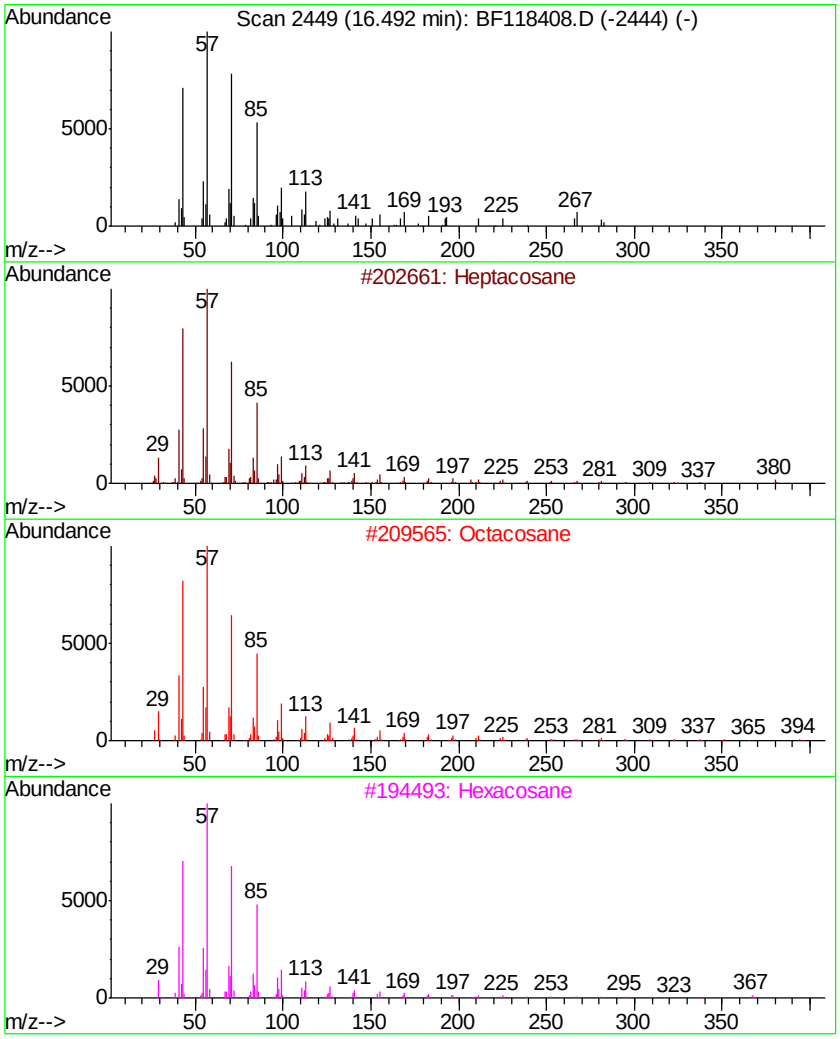
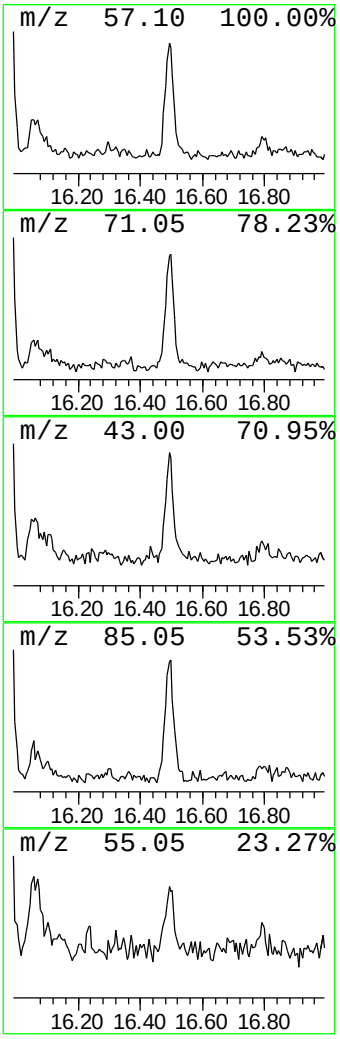
Peak Number 10 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.22 ng	82871	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Eicosane	282	C20H42	000112-95-8	87
5	Octadecane	254	C18H38	000593-45-3	87





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Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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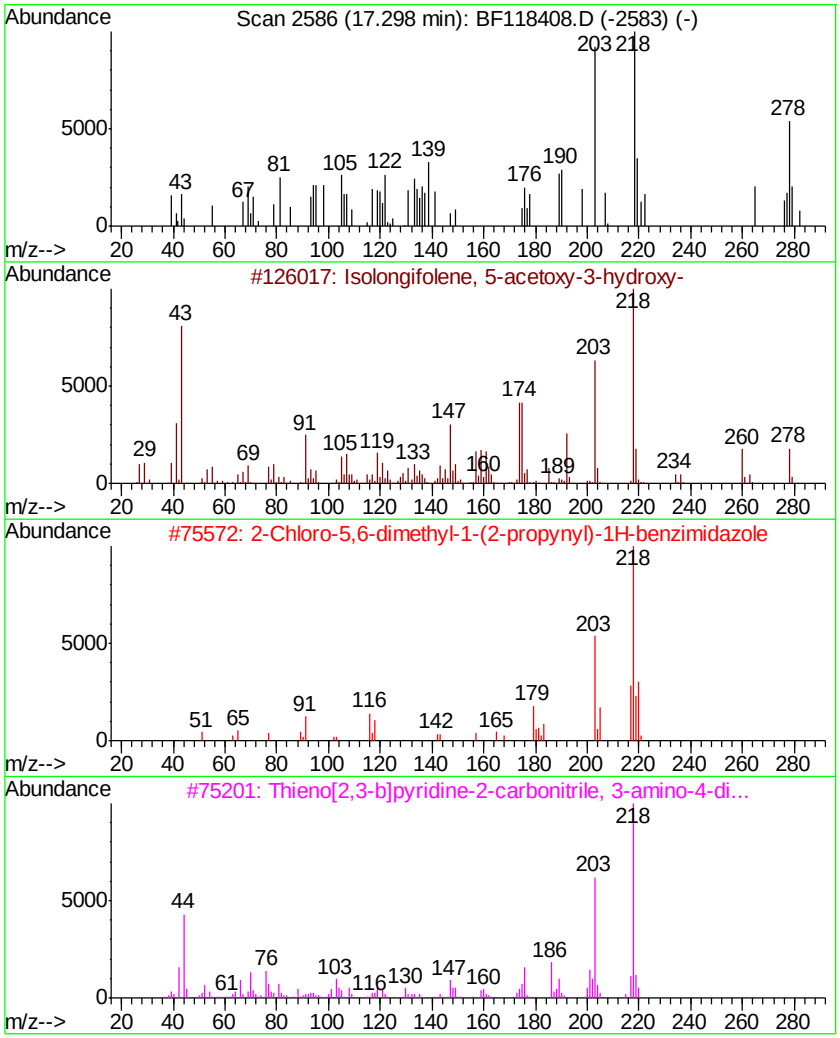
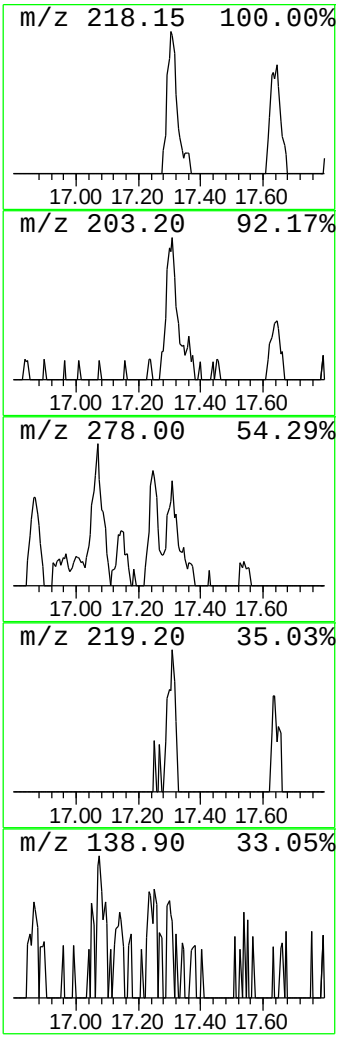
Peak Number 12 Isolongifolene, 5-acetoxy-3... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.44 ng	91175	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isolongifolene, 5-acetoxy-3-hydr...	278	C17H26O3	1000155-56-3	53
2	2-Chloro-5,6-dimethyl-1-(2-propy...	218	C12H11ClN2	080276-20-6	35
3	Thieno[2,3-b]pyridine-2-carbonit...	218	C10H10N4S	147992-88-9	35
4	4,4,9,9-Tetramethyl-4,9-disilatr...	218	C12H18Si2	1000280-67-7	35
5	Acetamide, N-2-[(4-chlorophenyl)...	304	C16H17ClN2O2	1000280-78-6	35





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Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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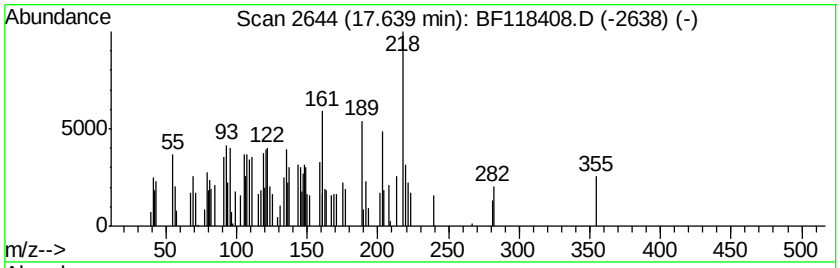
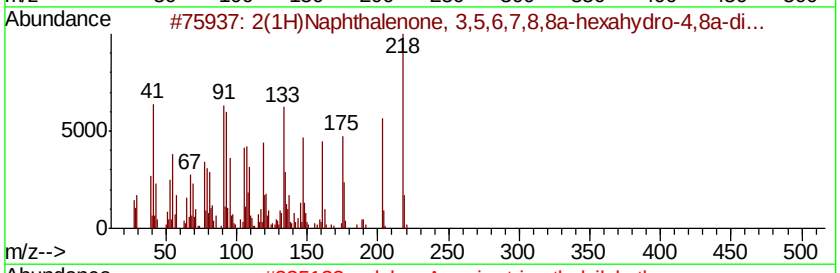
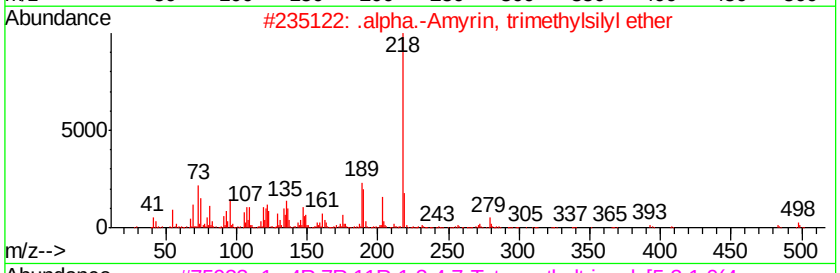
Peak Number 13 unknown17.64 Concentration Rank 9

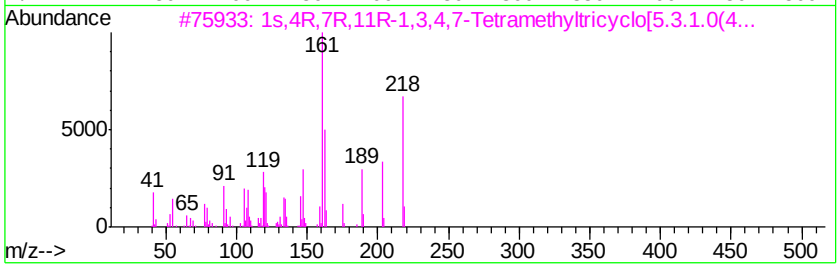
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	2.69 ng	100821	Perylene-d12	15.54

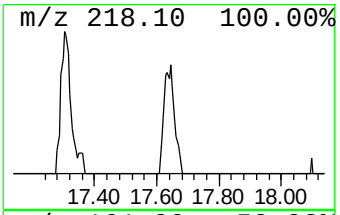
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	43
2	.alpha.-Amyrin, trimethylsilyl e...	498	C33H58OSi	1000374-76-6	38
3	1s,4R,7R,11R-1,3,4,7-Tetramethyl...	218	C15H22O	137235-42-8	30
4	2-(3,4-Methylenedioxyphenyl)cycl...	218	C13H14O3	042866-86-4	27
5	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	27

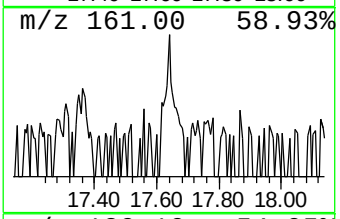


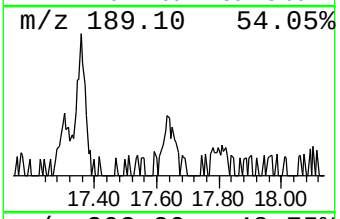


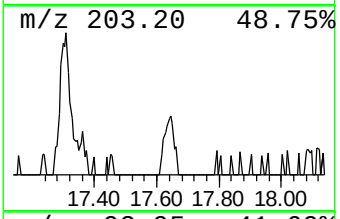


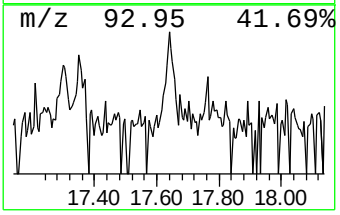












Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.06	11.6	ng	276916	1	6.85	478175	20.0
unknown6.62	6.62	74.4	ng	1779380	1	6.85	478175	20.0
n-Hexadecanoic acid	11.92	8.4	ng	333433	4	11.40	793549	20.0
1-Heneicosanol	13.88	9.8	ng	391660	5	14.05	795123	20.0
Heneicosane	14.50	2.4	ng	94650	5	14.05	795123	20.0
Eicosane	14.81	3.3	ng	122235	6	15.54	748262	20.0
Nonadecane, 9-met...	15.98	3.9	ng	145790	6	15.54	748262	20.0
1-Eicosene	16.06	2.3	ng	86953	6	15.54	748262	20.0
Heptacosane	16.49	2.2	ng	82871	6	15.54	748262	20.0
Isolongifolene, 5...	17.30	2.4	ng	91175	6	15.54	748262	20.0
unknown17.64	17.64	2.7	ng	100821	6	15.54	748262	20.0