LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115957.D
Acq On : 2 Aug 2019 20:04
Operator : HP/JU
Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

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-BF073019.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	5.469	571	575	600	rBV	2234306	2489560	73.50%	7.672%
2	6.481	743	747	767	rBV	2389082	2792054	82.43%	8.605%
3	6.622	767	771	774	rBV	3001328	2658506	78.49%	8.193%
4	6.851	806	810	819	rBV	895004	755987	22.32%	2.330%
5	7.010	833	837	840	rBV	2169181	2103086	62.09%	6.481%
6	7.410	901	905	908	rBV	1855207	1627182	48.04%	5.015%
7	8.134	1024	1028	1046	rBV	983355	973748	28.75%	3.001%
8	9.210	1207	1211	1223	rBV	3243512	2989070	88.25%	9.212%
9	9.604	1275	1278	1293	rBV	184914	182085	5.38%	0.561%
10	9.892	1323	1327	1342	rVB	1333812	1184932	34.98%	3.652%
11	10.681	1457	1461	1474	rBV	1994483	2011402	59.38%	6.199%
12	11.380	1576	1580	1582	rBV	1295408	1241980	36.67%	3.828%
13	11.404	1582	1584	1589	rVV	239128	220862	6.52%	0.681%
14	11.457	1589	1593	1596	rVB	55455	64678	1.91%	0.199%
15	11.880	1660	1665	1667	rBV	36279	34957	1.03%	0.108%
16	11.904	1667	1669	1676	rVV3	154838	182102	5.38%	0.561%
17	11.992	1681	1684	1687	rBV	70876	77628	2.29%	0.239%
18	12.427	1755	1758	1761	rBV	35837	36256	1.07%	0.112%
19	12.592	1782	1786	1790	rBV	634373	543710	16.05%	1.676%
20	12.692	1800	1803	1809	rBV3	43145	69291	2.05%	0.214%
21	12.822	1819	1825	1831	rBV	526665	583467	17.23%	1.798%
22	12.963	1842	1849	1852	rBV	3572638	3387186	100.00%	10.439%
23	13.151	1878	1881	1884	rVB	86217	78541	2.32%	0.242%
24	13.216	1889	1892	1895	rVV	60605	50936	1.50%	0.157%
25	13.251	1895	1898	1901	rBV2	44282	49322	1.46%	0.152%
26	13.533	1942	1946	1948	rBV4	43111	59958	1.77%	0.185%
27	13.769	1982	1986	1988	rBV	44567	49457	1.46%	0.152%
28	13.869	1999	2003	2020	rVB5	208237	607876	17.95%	1.873%
29	14.021	2021	2029	2031	rVV2	1367493	1524251	45.00%	4.697%
30	14.045	2031	2033	2042	rVB	281652	287827	8.50%	0.887%
31	14.127	2044	2047	2052	rVB	66470	64913	1.92%	0.200%
32	14.174	2052	2055	2058	rBV	48865	47420	1.40%	0.146%
33	14.410	2092	2095	2098	rVB	39806	35557	1.05%	0.110%
34	14.480	2103	2107	2110	rBV3	81386	83229	2.46%	0.256%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115957.D
Acq On : 2 Aug 2019 20:04
Operator : HP/JU
Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

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-BF073019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.551	2117	2119	2123	rVB	34167	34461	1.02%	0.106%
36	14.721	2140	2148	2154	rBV6	30171	80289	2.37%	0.247%
37	14.786	2156	2159	2165	rVV	100516	101648	3.00%	0.313%
38	14.863	2168	2172	2176	rVB	83350	87611	2.59%	0.270%
39	15.004	2186	2196	2199	rBV5	48645	153942	4.54%	0.474%
40	15.063	2202	2206	2209	rVV	202107	345044	10.19%	1.063%
41	15.121	2213	2216	2221	rVB3	145060	208091	6.14%	0.641%
42	15.363	2254	2257	2264	rVB	94903	135961	4.01%	0.419%
43	15.427	2264	2268	2273	rVV	157271	219216	6.47%	0.676%
44	15.492	2273	2279	2294	rVB	854681	1320639	38.99%	4.070%
45	15.939	2349	2355	2360	rBV	110728	172750	5.10%	0.532%
46	16.439	2435	2440	2449	rBV3	63056	131508	3.88%	0.405%
47	16.968	2524	2530	2537	rBV	58674	122060	3.60%	0.376%
48	17.033	2537	2541	2548	rVB6	36158	69565	2.05%	0.214%
49	17.409	2600	2605	2622	rVB	44416	116936	3.45%	0.360%

Sum of corrected areas: 32448737

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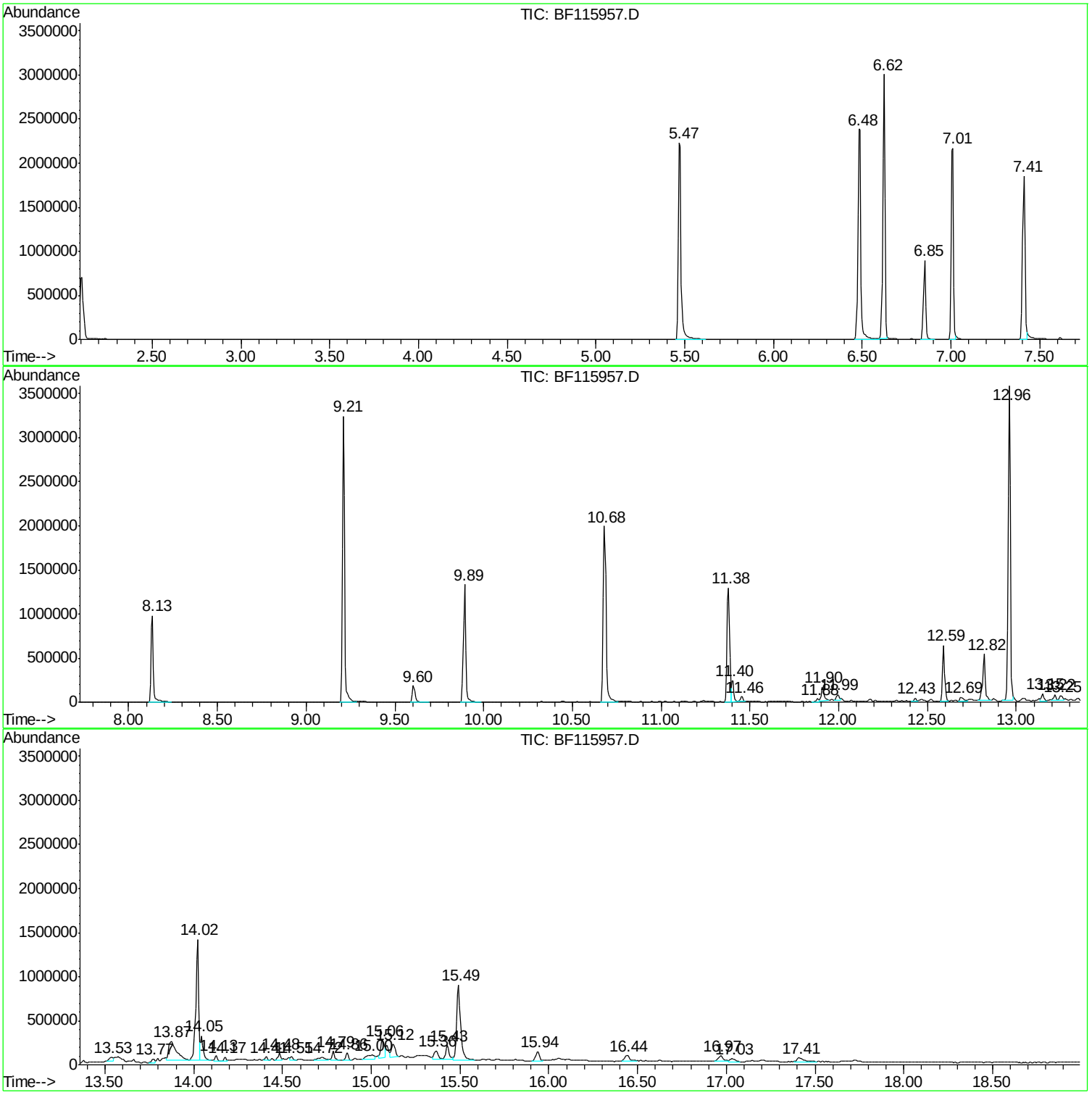
Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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\BF080219\
Data File : BF115957.D
Acq On : 2 Aug 2019 20:04
Operator : HP/JU
Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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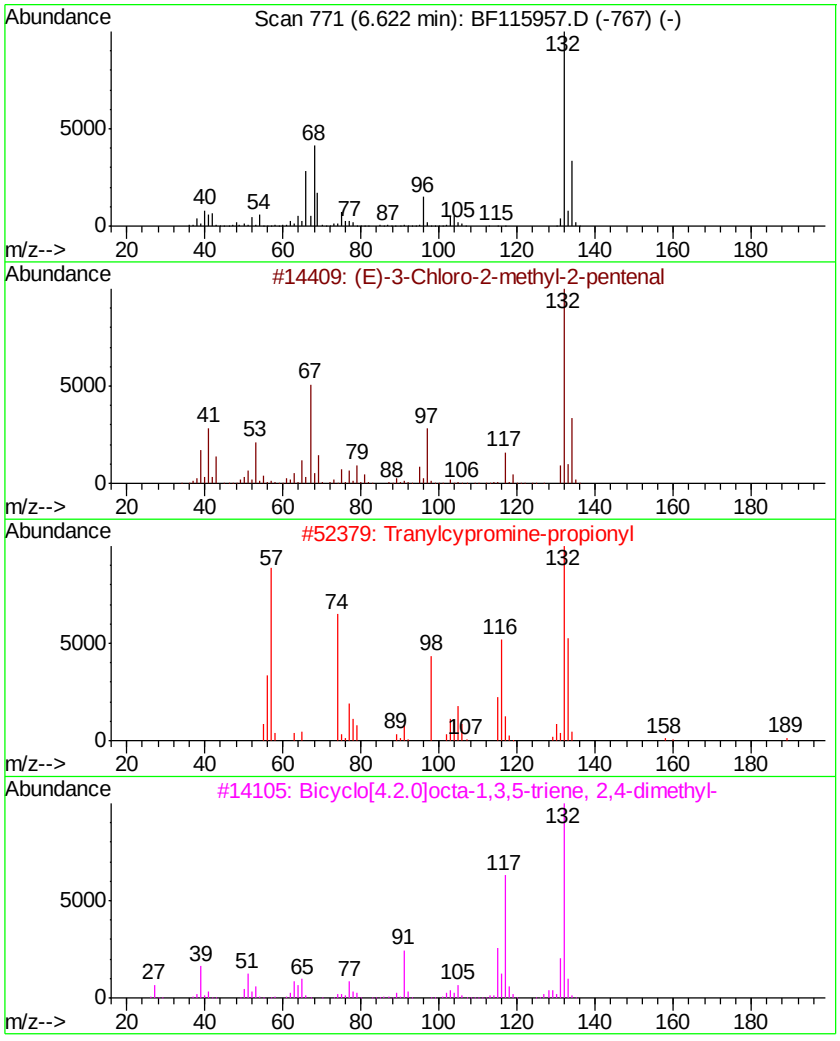
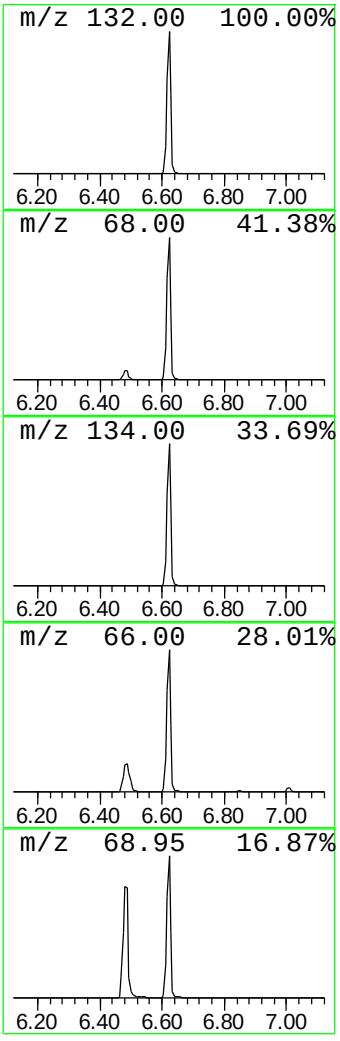
Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	70.33 ng	2658510	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Xenon	132	Xe	007440-63-3	9





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Data File : BF115957.D
Acq On : 2 Aug 2019 20:04
Operator : HP/JU
Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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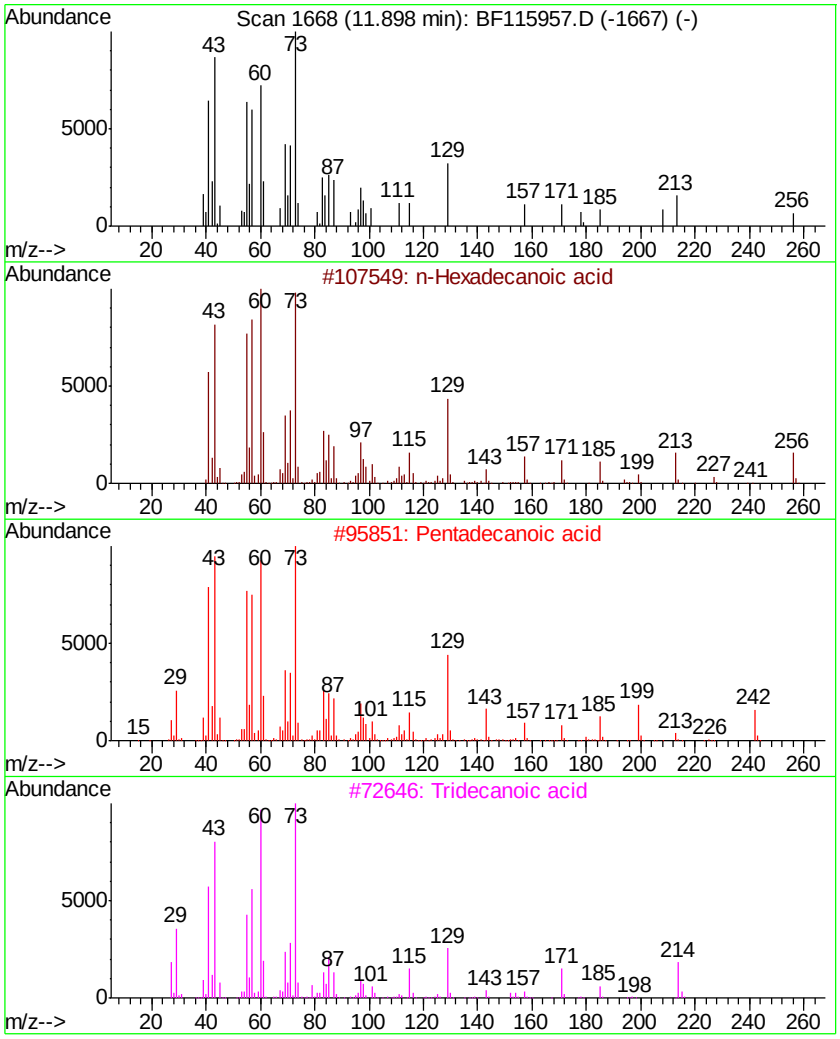
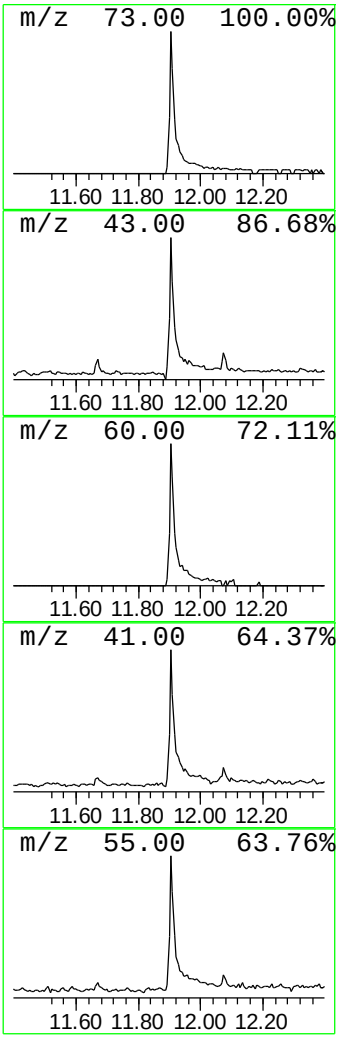
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.93 ng	182102	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	25
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	20





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115957.D
Acq On : 2 Aug 2019 20:04
Operator : HP/JU
Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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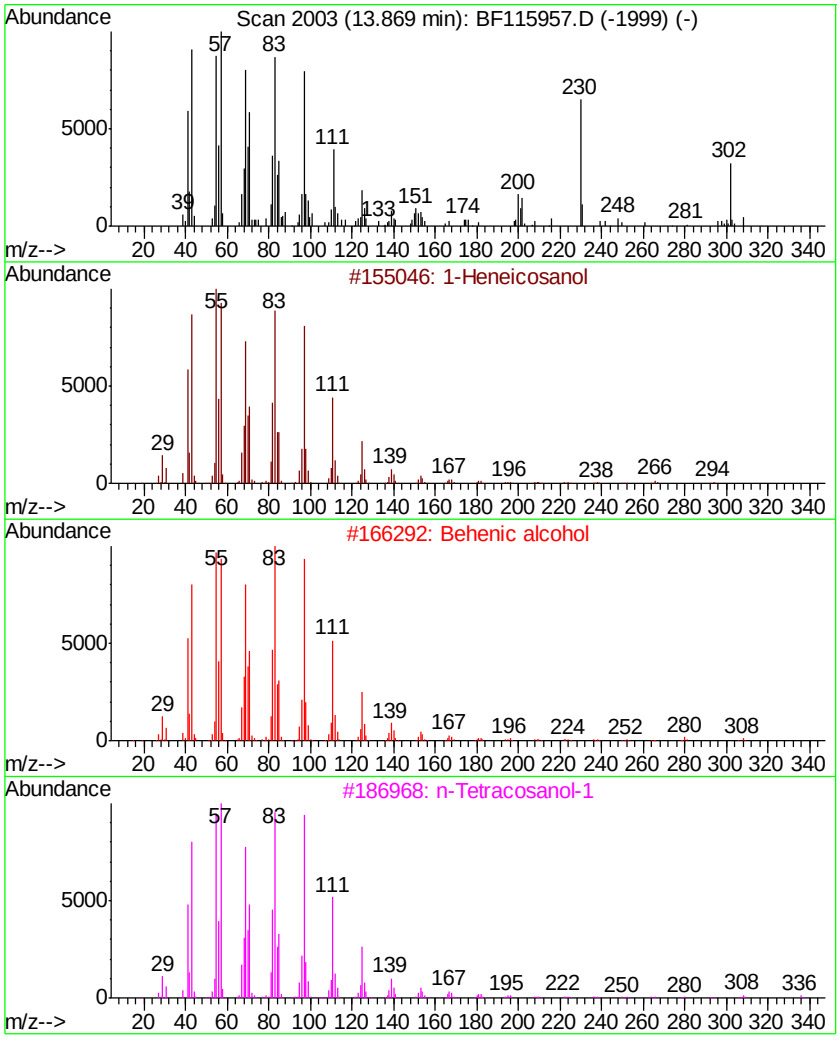
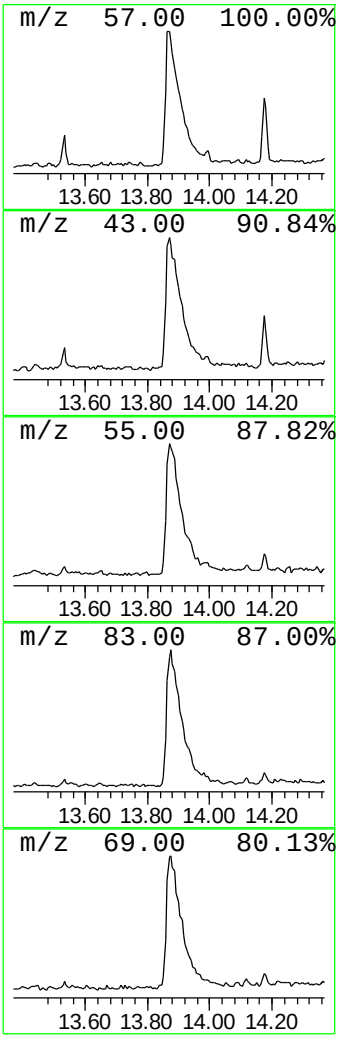
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	7.98 ng	607876	Chrysene-d12	14.02

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	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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Data File : BF115957.D
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Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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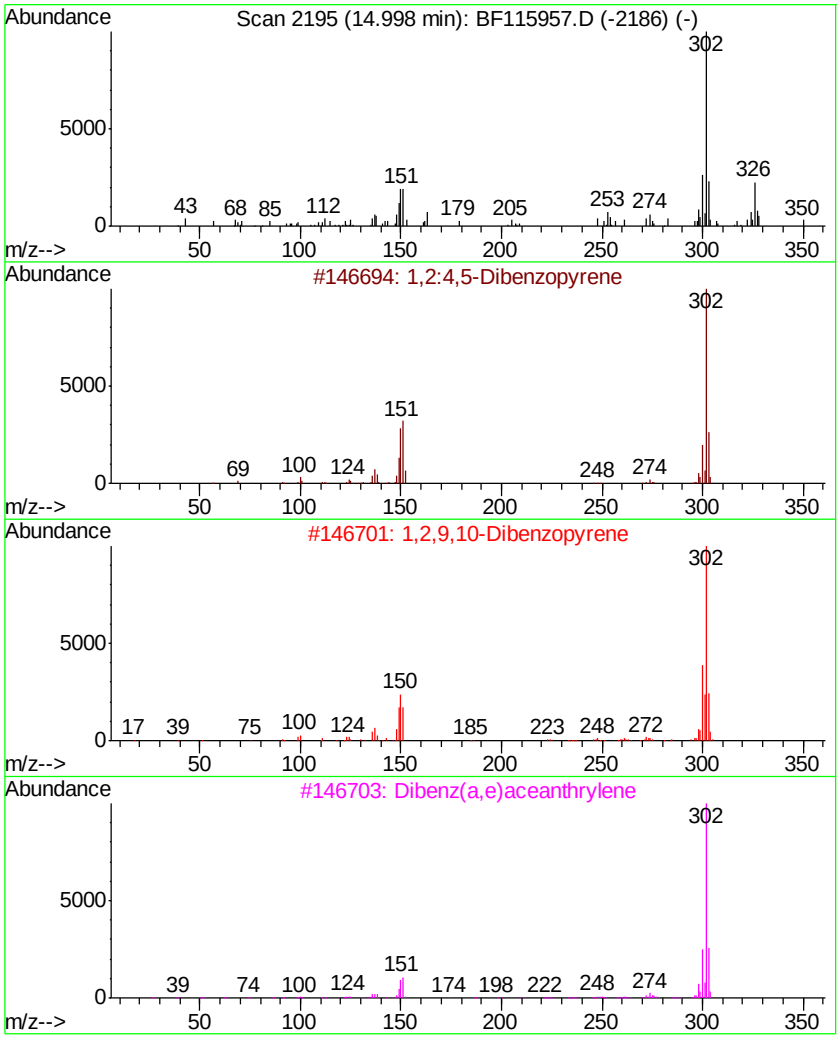
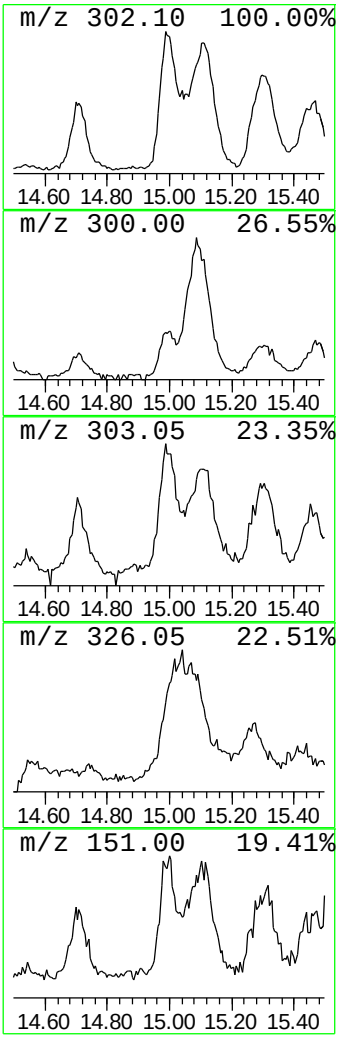
Peak Number 5 1,2:4,5-Dibenzopyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.33 ng	153942	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	64
2	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	60
3	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	60
4	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	53
5	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	53





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Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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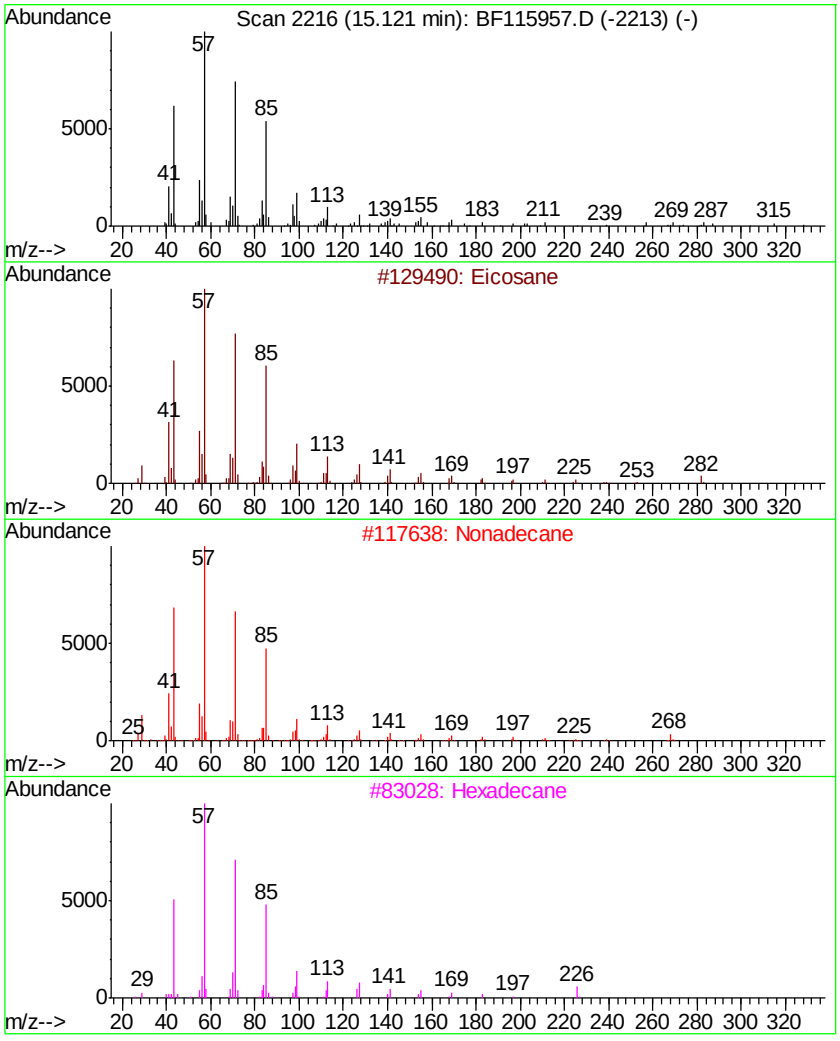
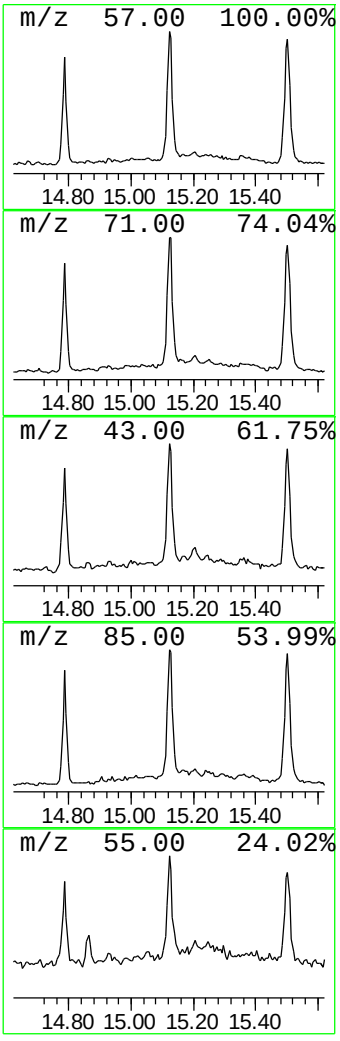
Peak Number 6 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	3.15 ng	208091	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Nonadecane	268	C19H40	000629-92-5	93
3	Hexadecane	226	C16H34	000544-76-3	93
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115957.D
Acq On : 2 Aug 2019 20:04
Operator : HP/JU
Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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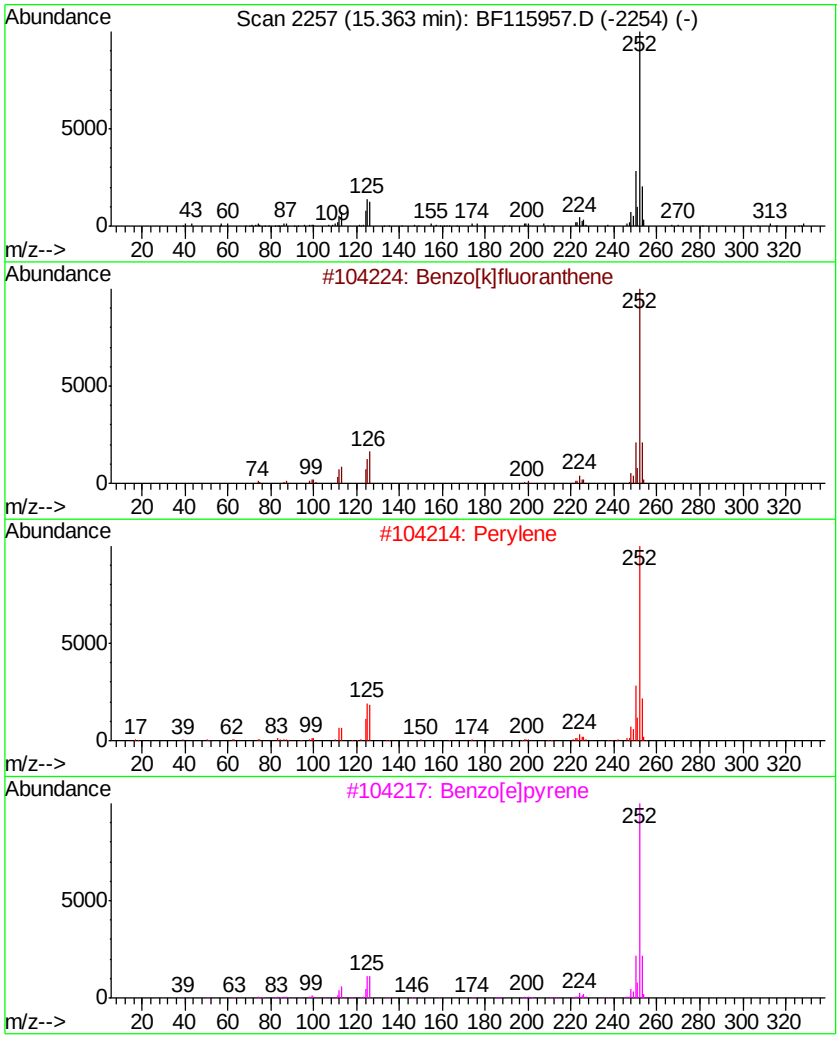
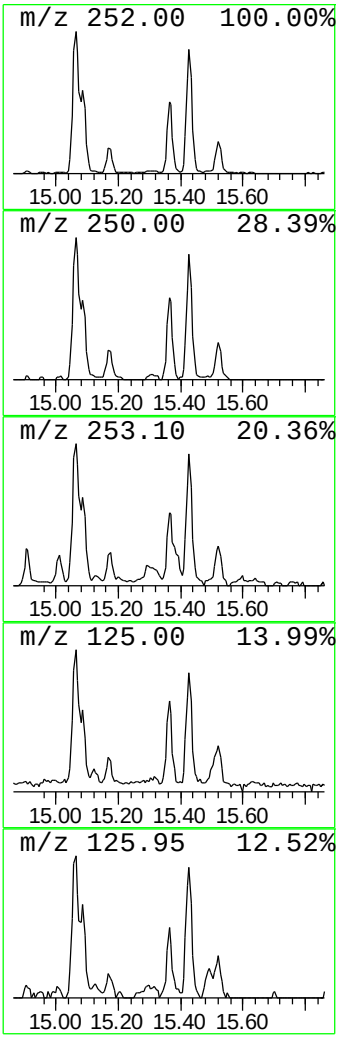
Peak Number 7 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.06 ng	135961	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[e]pyrene	252	C20H12	000192-97-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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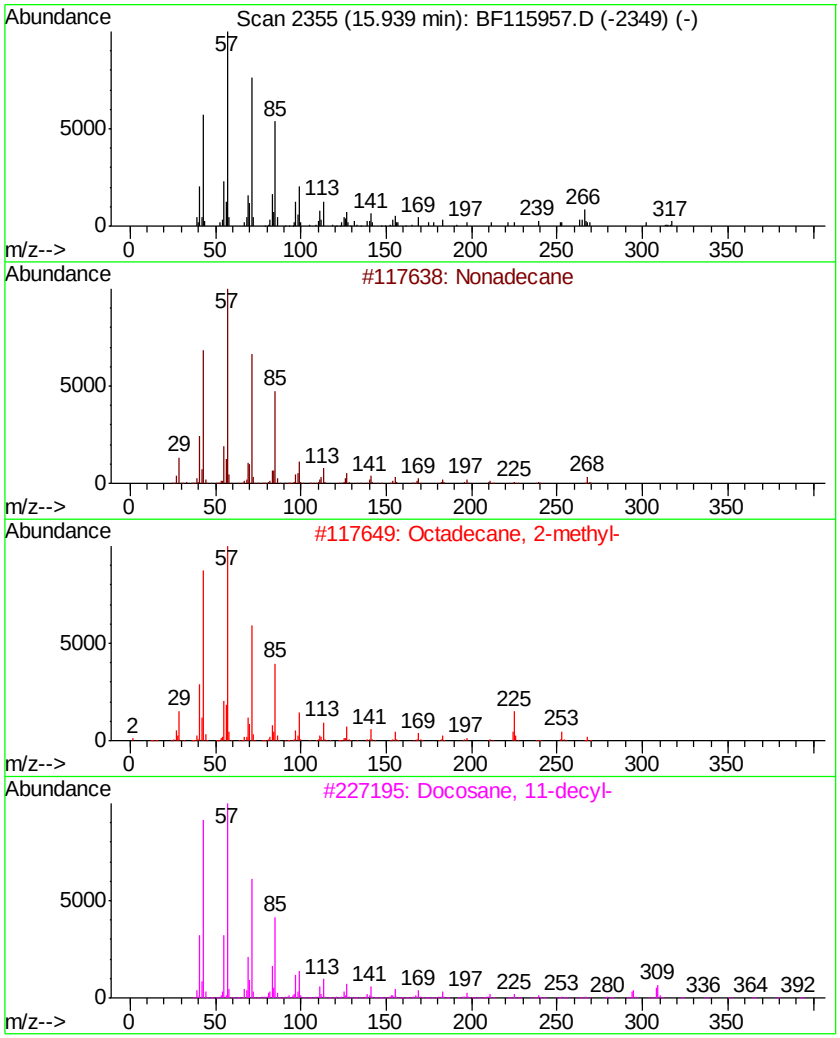
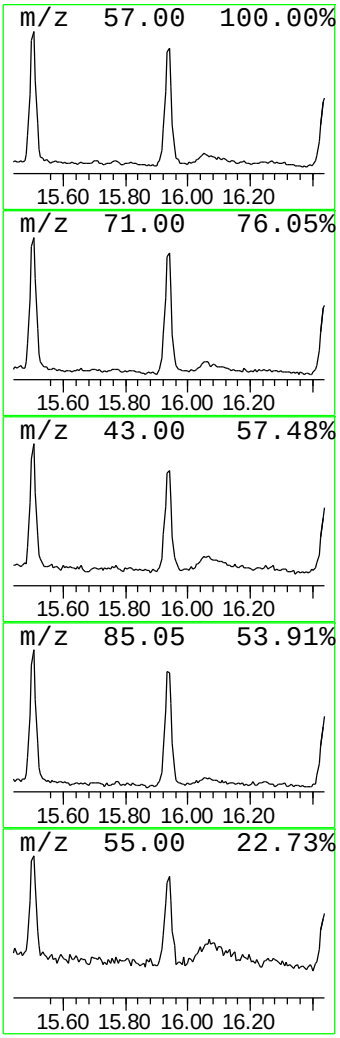
Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.62 ng	172750	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Octacosane	394	C28H58	000630-02-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080219\
Data File : BF115957.D
Acq On : 2 Aug 2019 20:04
Operator : HP/JU
Sample : K4130-14
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1S-L-(0-30)-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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
unknown6.62	6.62	70.3	ng	2658510	1	6.85	755987	20.0
n-Hexadecanoic acid	11.90	2.9	ng	182102	4	11.38	1241980	20.0
1-Heneicosanol	13.87	8.0	ng	607876	5	14.02	1524250	20.0
1,2:4,5-Dibenzopy...	15.00	2.3	ng	153942	6	15.49	1320640	20.0
Eicosane	15.12	3.1	ng	208091	6	15.49	1320640	20.0
Perylene	15.36	2.1	ng	135961	6	15.49	1320640	20.0
Nonadecane	15.94	2.6	ng	172750	6	15.49	1320640	20.0