LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115968.D
Acq On : 3 Aug 2019 1:00
Operator : HP/JU
Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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	3.905	303	309	325	rVB	739243	1044279	45.22%	5.583%
2	5.469	572	575	599	rBV	261915	334648	14.49%	1.789%
3	6.481	744	747	767	rBV2	234219	432784	18.74%	2.314%
4	6.622	767	771	780	rBV	758460	701529	30.37%	3.750%
5	6.851	806	810	818	rBV	872100	731366	31.67%	3.910%
6	7.004	833	836	852	rVB	1453067	1386393	60.03%	7.412%
7	7.263	874	880	891	rBV	50082	93093	4.03%	0.498%
8	7.410	901	905	917	rBV	1222354	1102531	47.74%	5.894%
9	7.922	986	992	997	rBV5	16224	33972	1.47%	0.182%
10	8.134	1024	1028	1043	rBV	1057648	979237	42.40%	5.235%
11	8.934	1161	1164	1176	rBV3	30607	61407	2.66%	0.328%
12	9.210	1207	1211	1222	rBV	2435405	2103256	91.07%	11.244%
13	9.604	1275	1278	1284	rBV	150815	134950	5.84%	0.721%
14	9.892	1319	1327	1334	rBV	1399092	1220068	52.83%	6.523%
15	9.957	1334	1338	1345	rVB6	12242	25014	1.08%	0.134%
16	10.269	1388	1391	1398	rBV4	31887	58105	2.52%	0.311%
17	10.681	1457	1461	1469	rBV	633880	637522	27.60%	3.408%
18	11.380	1576	1580	1587	rBV	1366377	1262817	54.68%	6.751%
19	11.463	1591	1594	1599	rVV3	21822	35760	1.55%	0.191%
20	11.833	1654	1657	1659	rBV	38503	32879	1.42%	0.176%
21	11.904	1666	1669	1676	rBV2	177309	218939	9.48%	1.170%
22	12.057	1692	1695	1702	rVB2	40099	40009	1.73%	0.214%
23	12.692	1799	1803	1812	rBV	55515	88257	3.82%	0.472%
24	12.963	1845	1849	1852	rBV	2572976	2309567	100.00%	12.347%
25	13.863	1998	2002	2017	rBV	149046	354945	15.37%	1.898%
26	13.992	2022	2024	2026	rVV	36528	35867	1.55%	0.192%
27	14.021	2026	2029	2039	rVB	1057076	980534	42.46%	5.242%
28	14.180	2052	2056	2058	rBV	45090	46085	2.00%	0.246%
29	14.480	2104	2107	2110	rBV	94700	85727	3.71%	0.458%
30	14.786	2155	2159	2163	rVB	141729	139922	6.06%	0.748%
31	14.863	2169	2172	2179	rVB	41752	39196	1.70%	0.210%
32	15.127	2212	2217	2225	rVB	147006	178948	7.75%	0.957%
33	15.492	2274	2279	2293	rBV	822936	1225681	53.07%	6.553%
34	15.933	2350	2354	2363	rBV	113777	177147	7.67%	0.947%

LSC Area Percent Report

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Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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	16.386	2426	2431	2435	rBV7	37064	86809	3.76%	0.464%
36	16.439	2436	2440	2452	rVB3	86578	189278	8.20%	1.012%
37	16.727	2486	2489	2498	rVB8	19592	34769	1.51%	0.186%
38	17.027	2538	2540	2548	rVB3	35039	62134	2.69%	0.332%

Sum of corrected areas: 18705424

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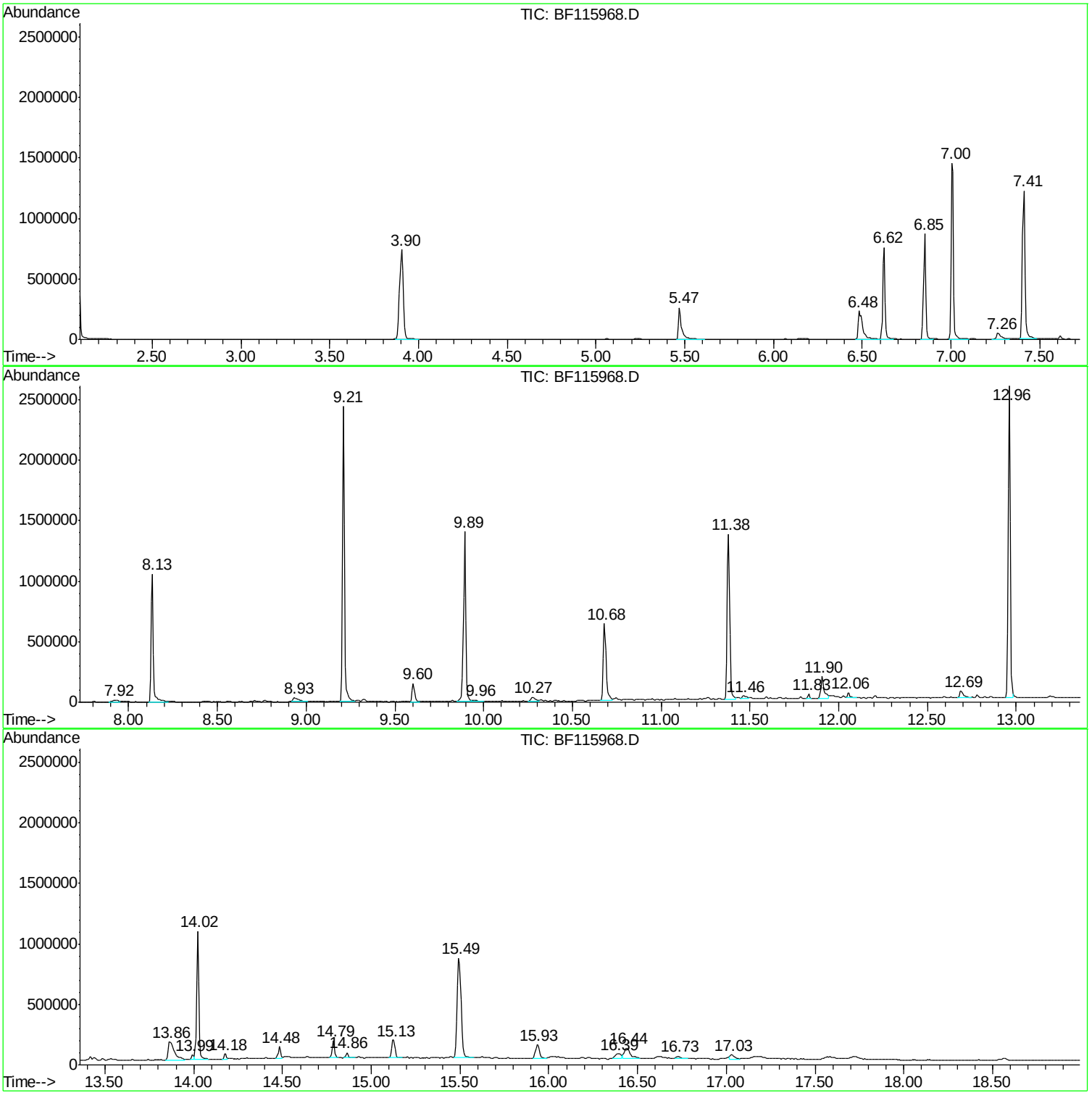
Instrument :
BNA_F
ClientSampleId :
CS-TEST-PIT

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



Library Search Compound Report

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Data File : BF115968.D
Acq On : 3 Aug 2019 1:00
Operator : HP/JU
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

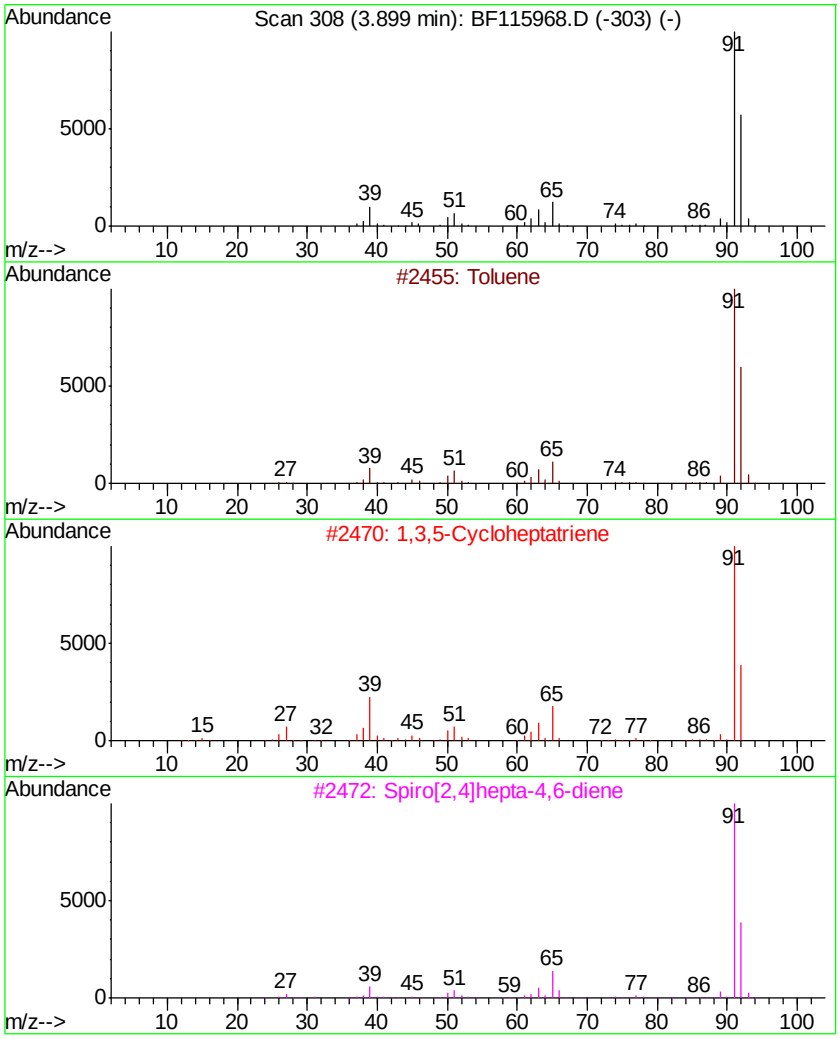
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

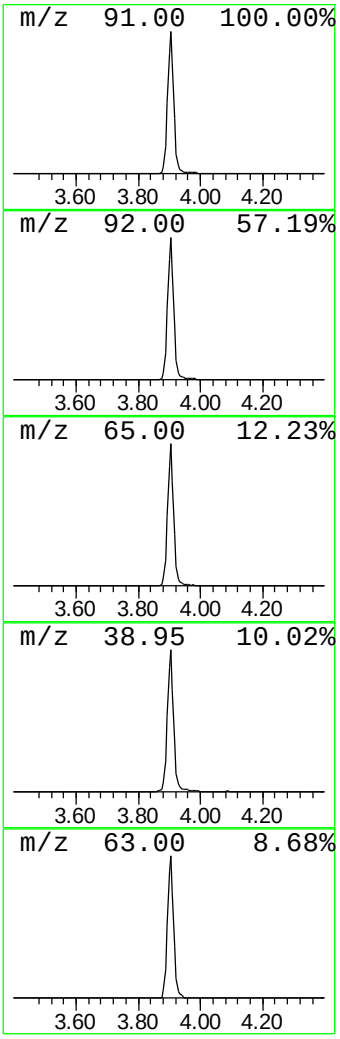
****

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.90	28.56 ng	1044280	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	95
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	87
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	78
5	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115968.D
Acq On : 3 Aug 2019 1:00
Operator : HP/JU
Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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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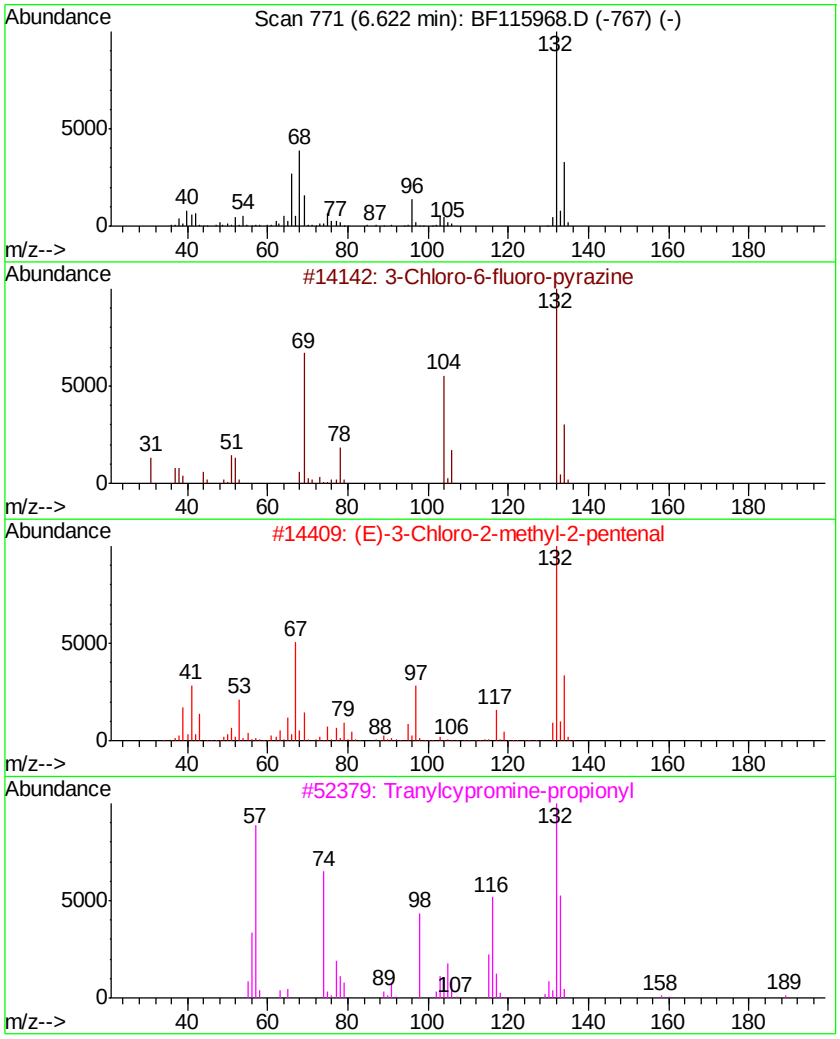
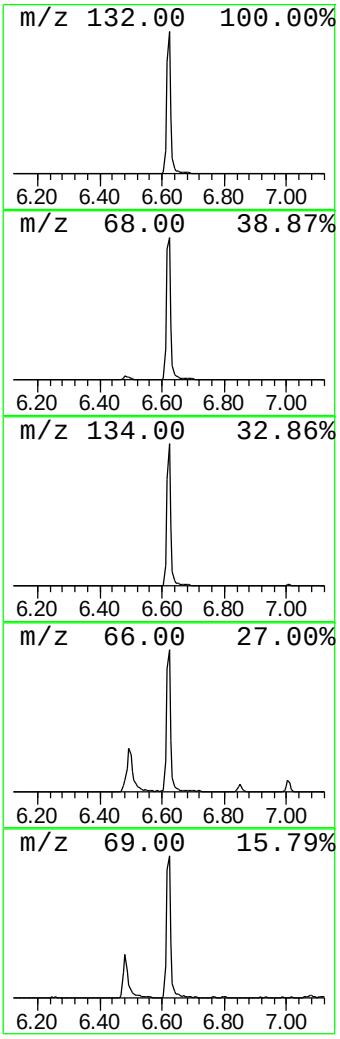
Peak Number 2 unknown6.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	19.18 ng	701529	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	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\BF080219\
Data File : BF115968.D
Acq On : 3 Aug 2019 1:00
Operator : HP/JU
Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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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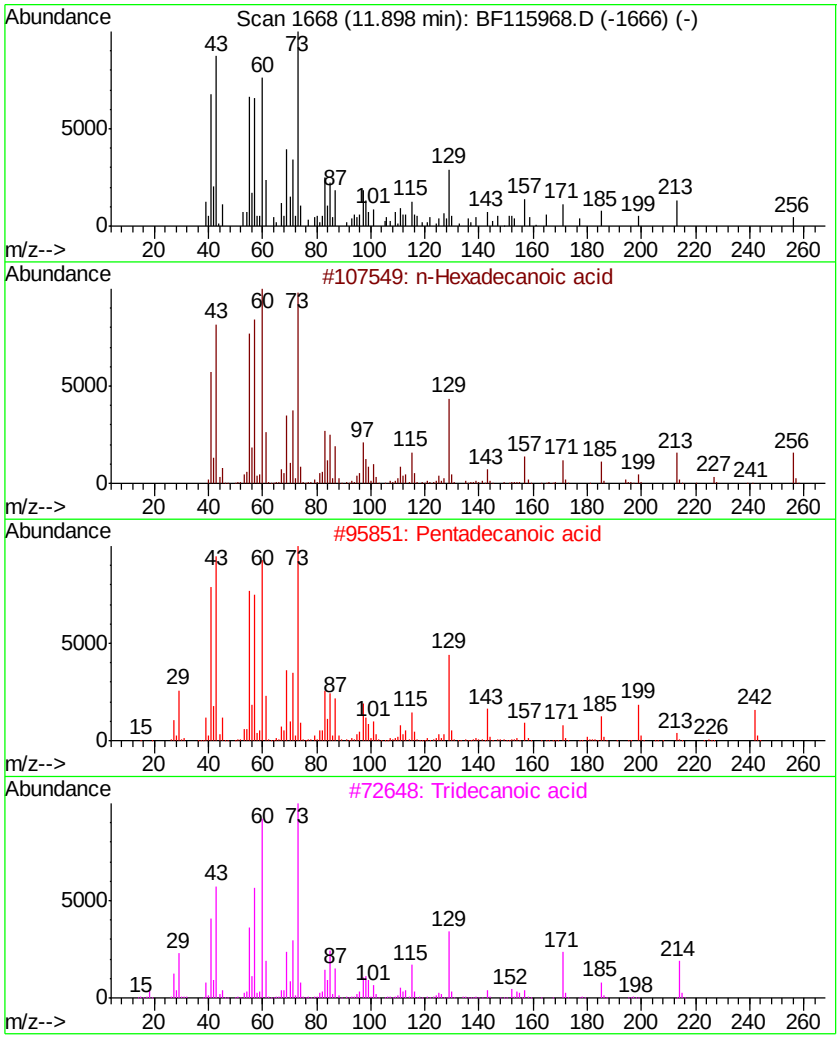
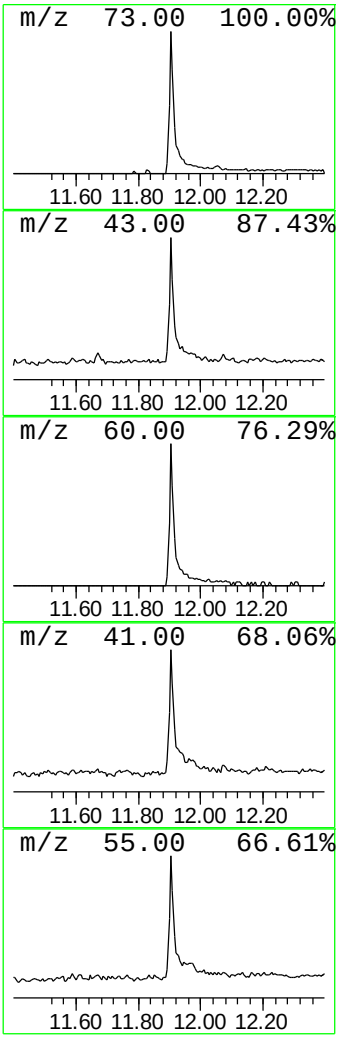
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.47 ng	218939	Phenanthrene-d10	11.38

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080219\
Data File : BF115968.D
Acq On : 3 Aug 2019 1:00
Operator : HP/JU
Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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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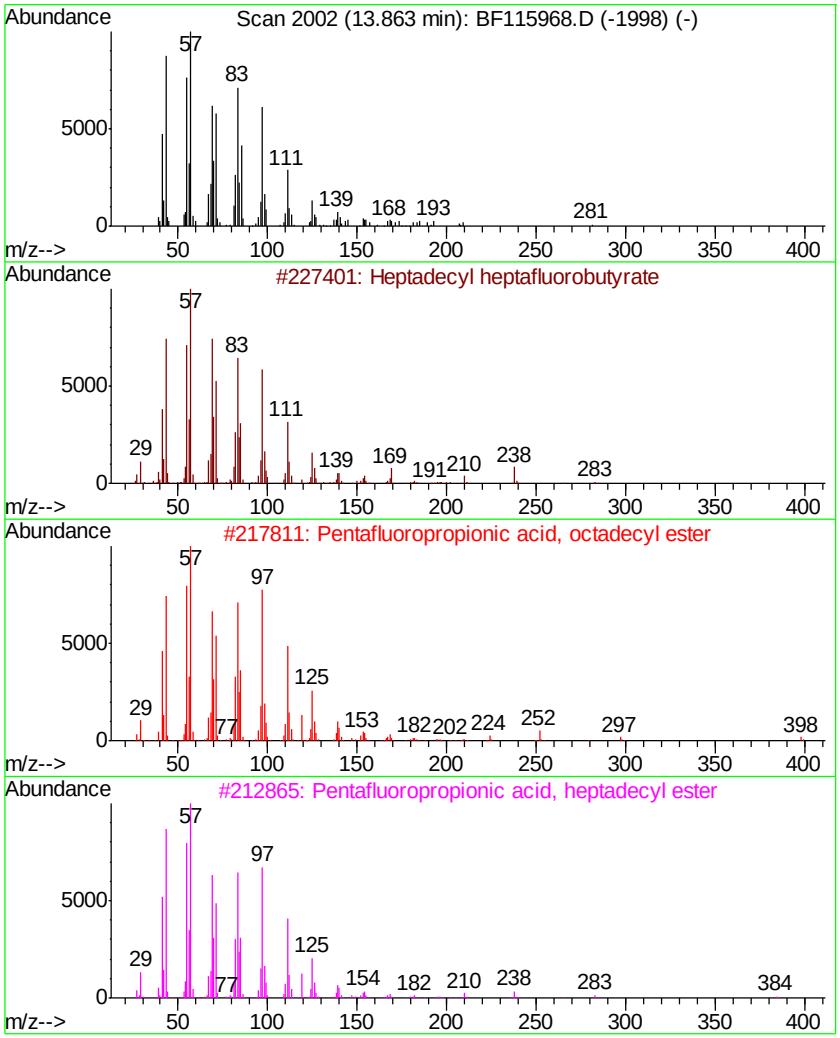
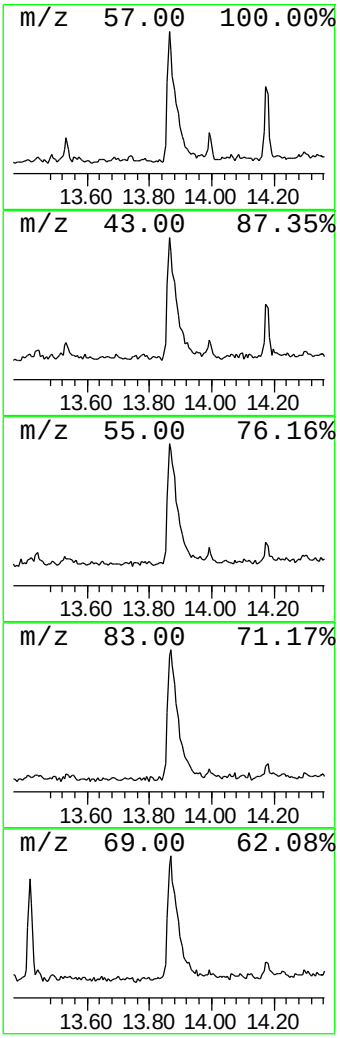
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	7.24 ng	354945	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	81
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	81





Library Search Compound Report

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Data File : BF115968.D
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Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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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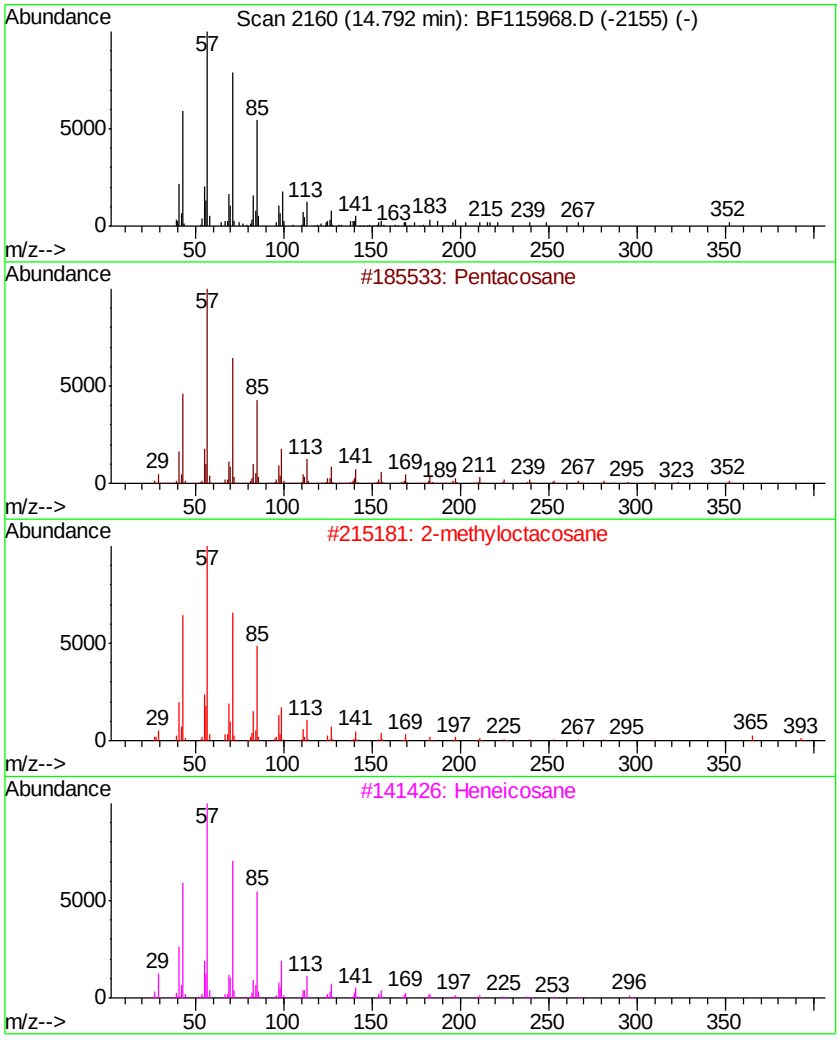
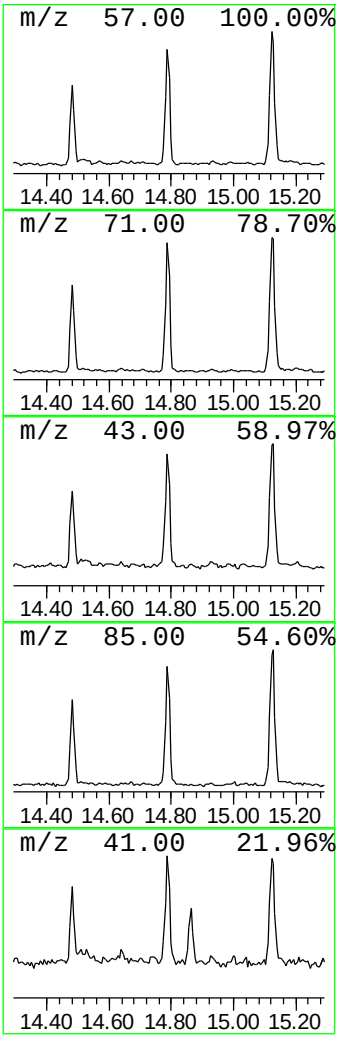
Peak Number 6 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.28 ng	139922	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
5	Hexacosane	366	C26H54	000630-01-3	90





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Sample : K4114-01
Misc :
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Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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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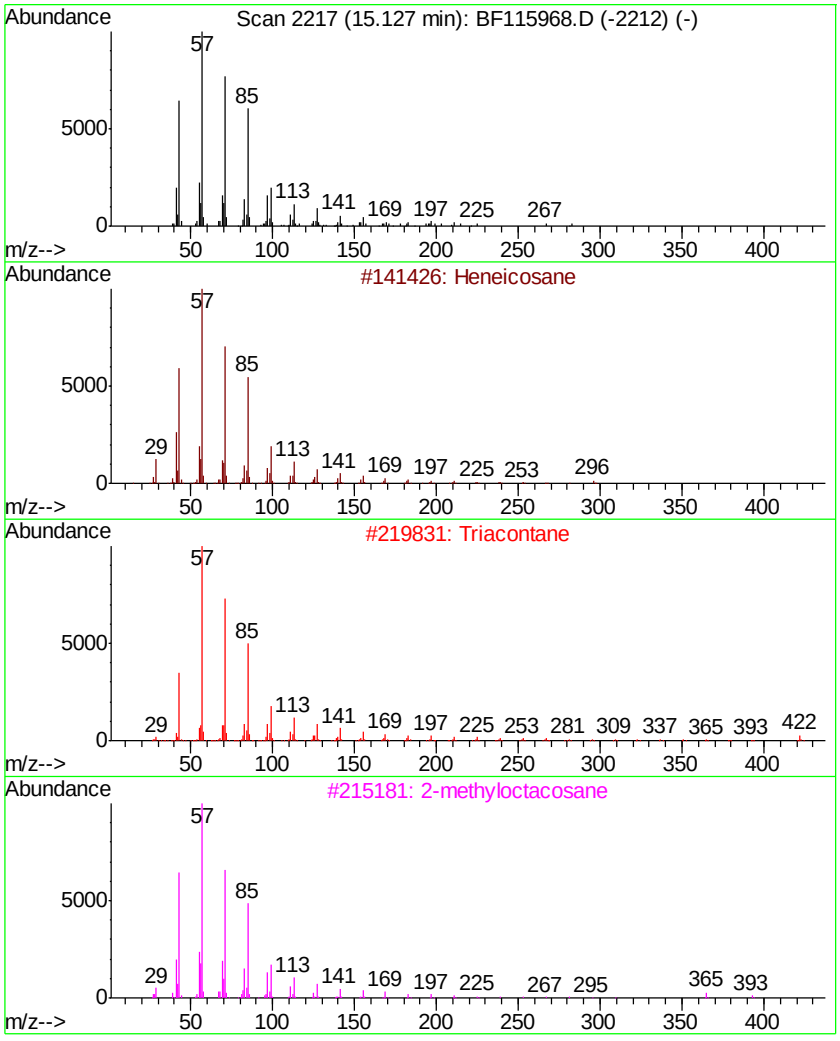
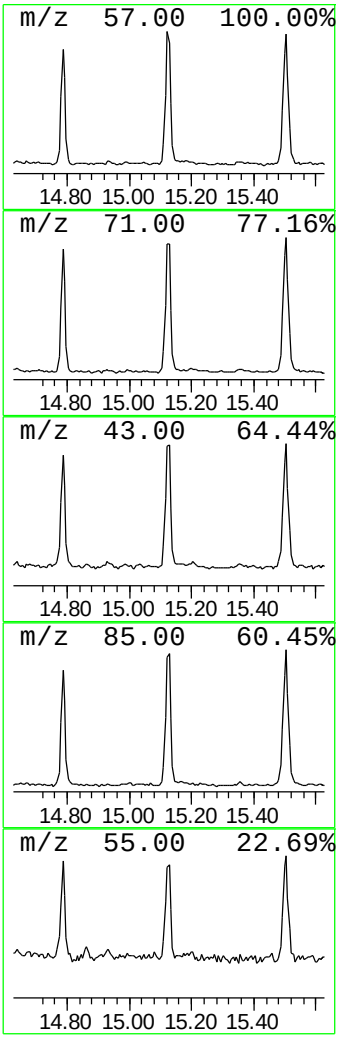
Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	2.92 ng	178948	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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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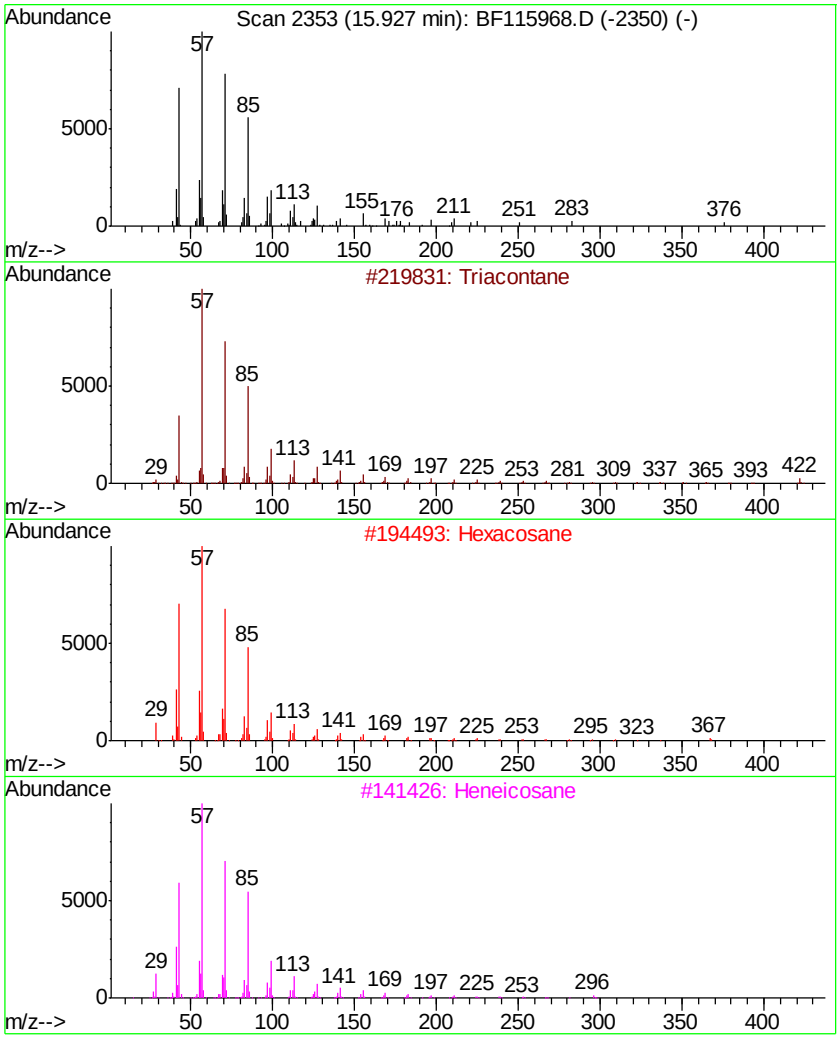
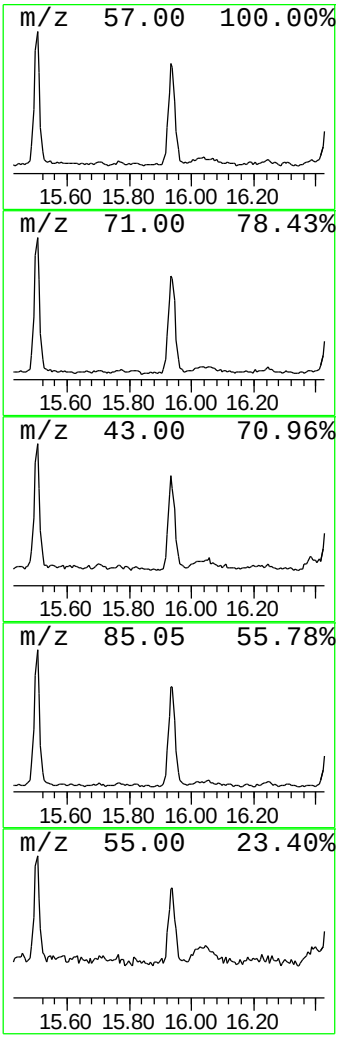
Peak Number 8 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.89 ng	177147	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Octadecane	254	C18H38	000593-45-3	87





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Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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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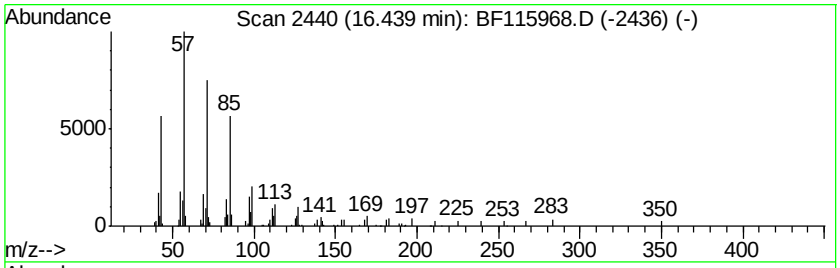
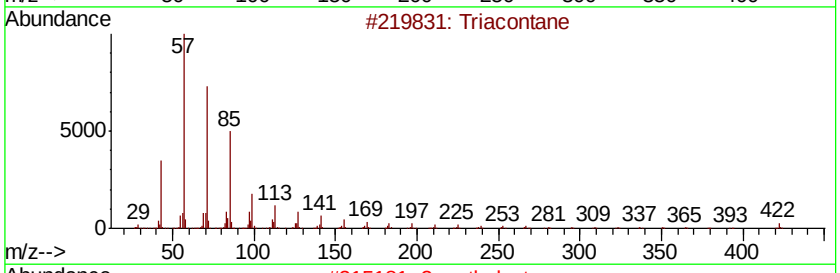
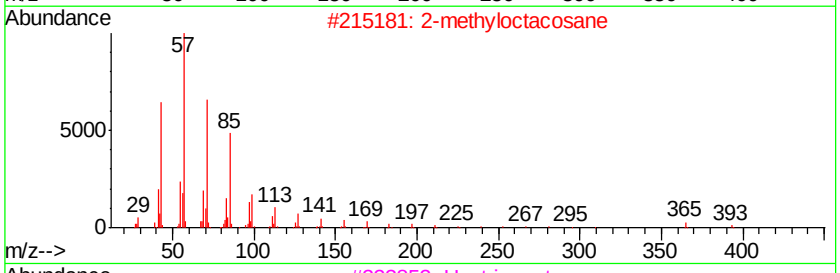
Peak Number 9 2-methyloctacosane Concentration Rank 6

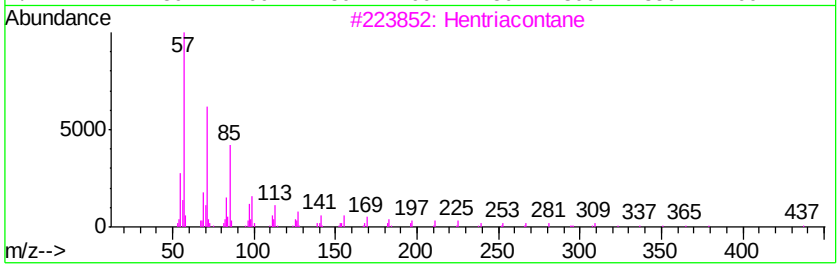
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	3.09 ng	189278	Perylene-d12	15.49

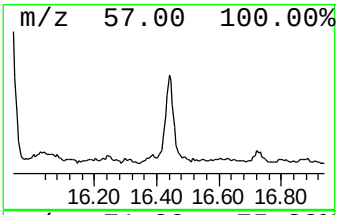
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Hexatriacontane	507	C36H74	000630-06-8	90

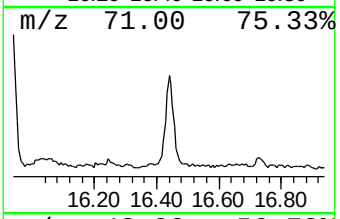


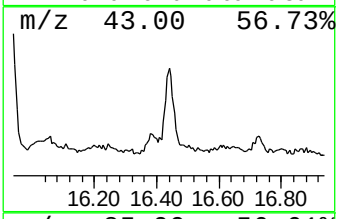


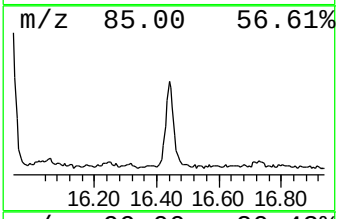


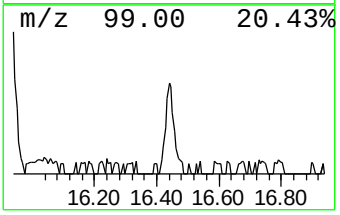












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080219\
Data File : BF115968.D
Acq On : 3 Aug 2019 1:00
Operator : HP/JU
Sample : K4114-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-TEST-PIT

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
1,3,5-Cycloheptat...	3.90	28.6	ng	1044280	1	6.85	731366	20.0
unknown6.62	6.62	19.2	ng	701529	1	6.85	731366	20.0
n-Hexadecanoic acid	11.90	3.5	ng	218939	4	11.38	1262820	20.0
Heptadecyl heptaf...	13.86	7.2	ng	354945	5	14.02	980534	20.0
Pentacosane	14.79	2.3	ng	139922	6	15.49	1225680	20.0
Heneicosane	15.13	2.9	ng	178948	6	15.49	1225680	20.0
Triacontane	15.93	2.9	ng	177147	6	15.49	1225680	20.0
2-methyloctacosane	16.44	3.1	ng	189278	6	15.49	1225680	20.0