LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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	5.457	570	573	606	rBV	1393621	1571378	29.89%	4.181%
2	6.469	742	745	765	rBV	1194700	1317442	25.06%	3.506%
3	6.610	765	769	778	rBV	3031765	2770037	52.70%	7.371%
4	6.834	804	807	816	rBV	827094	781770	14.87%	2.080%
5	6.904	816	819	830	rVV	32805	57897	1.10%	0.154%
6	6.992	830	834	849	rVB	2846490	2656599	50.54%	7.069%
7	7.245	874	877	887	rVB	74468	79120	1.51%	0.211%
8	7.398	899	903	916	rVB	2104113	2162177	41.13%	5.753%
9	8.116	1022	1025	1044	rVB	1073360	981136	18.67%	2.611%
10	9.192	1203	1208	1211	rBV	4264765	3964611	75.42%	10.550%
11	9.586	1271	1275	1280	rBV	131219	130991	2.49%	0.349%
12	9.869	1319	1323	1333	rVB	1389080	1222644	23.26%	3.253%
13	10.251	1385	1388	1390	rBV	68791	57480	1.09%	0.153%
14	10.280	1390	1393	1399	rVB	79333	95164	1.81%	0.253%
15	10.663	1453	1458	1474	rBV	2495307	2605281	49.56%	6.932%
16	11.357	1572	1576	1584	rBV	1431829	1339145	25.48%	3.563%
17	11.422	1584	1587	1592	rVB3	74330	69629	1.32%	0.185%
18	11.880	1661	1665	1669	rBV	409595	470003	8.94%	1.251%
19	12.580	1779	1784	1791	rBV3	38219	97658	1.86%	0.260%
20	12.669	1793	1799	1812	rVV	457246	728880	13.87%	1.939%
21	12.810	1819	1823	1825	rBV	77247	74805	1.42%	0.199%
22	12.945	1840	1846	1849	rBV	4708427	5256420	100.00%	13.987%
23	13.163	1880	1883	1887	rBV	139397	125683	2.39%	0.334%
24	13.410	1921	1925	1931	rVB3	47016	75655	1.44%	0.201%
25	13.504	1937	1941	1944	rBV2	226594	205200	3.90%	0.546%
26	13.833	1993	1997	2012	rBV	564835	812248	15.45%	2.161%
27	13.998	2021	2025	2034	rVB	1470126	1487108	28.29%	3.957%
28	14.145	2046	2050	2054	rBV	480883	484665	9.22%	1.290%
29	14.451	2098	2102	2106	rBV	653241	605129	11.51%	1.610%
30	14.757	2149	2154	2162	rBV	677068	746284	14.20%	1.986%
31	14.827	2162	2166	2171	rVB	215085	212824	4.05%	0.566%
32	15.086	2205	2210	2219	rVB	671467	785770	14.95%	2.091%
33	15.457	2267	2273	2287	rBV2	1454699	2067027	39.32%	5.500%
34	15.886	2339	2346	2353	rBV	424190	664953	12.65%	1.769%

LSC Area Percent Report

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Data File : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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	15.974	2356	2361	2373	rVB10	22467	83352	1.59%	0.222%
36	16.380	2423	2430	2449	rVB	240193	496261	9.44%	1.321%
37	16.956	2522	2528	2537	rVB	61854	129033	2.45%	0.343%
38	17.498	2613	2620	2631	rBV10	30513	109447	2.08%	0.291%

Sum of corrected areas: 37580906

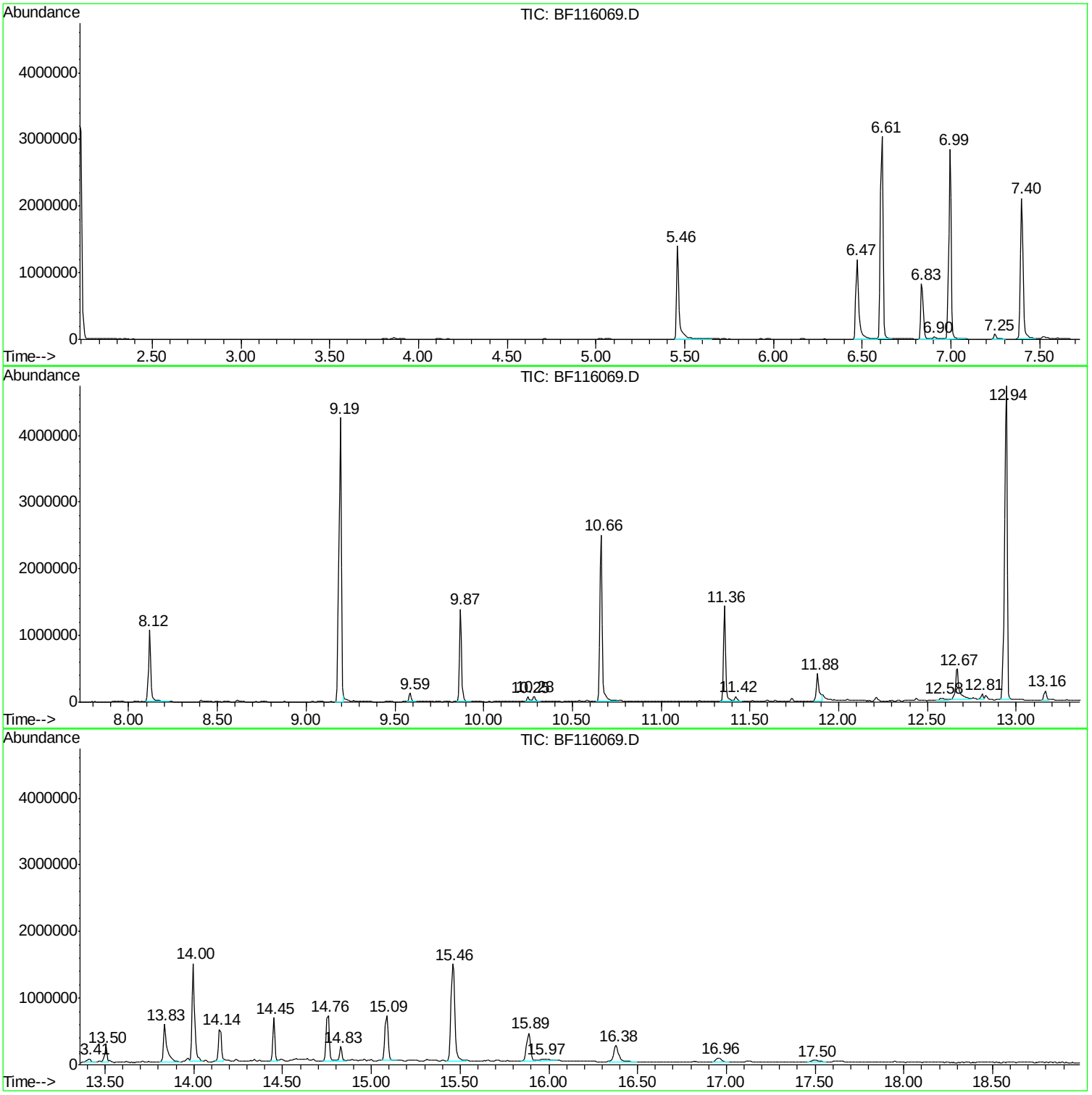
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-BH-1-ELU-20190610

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 : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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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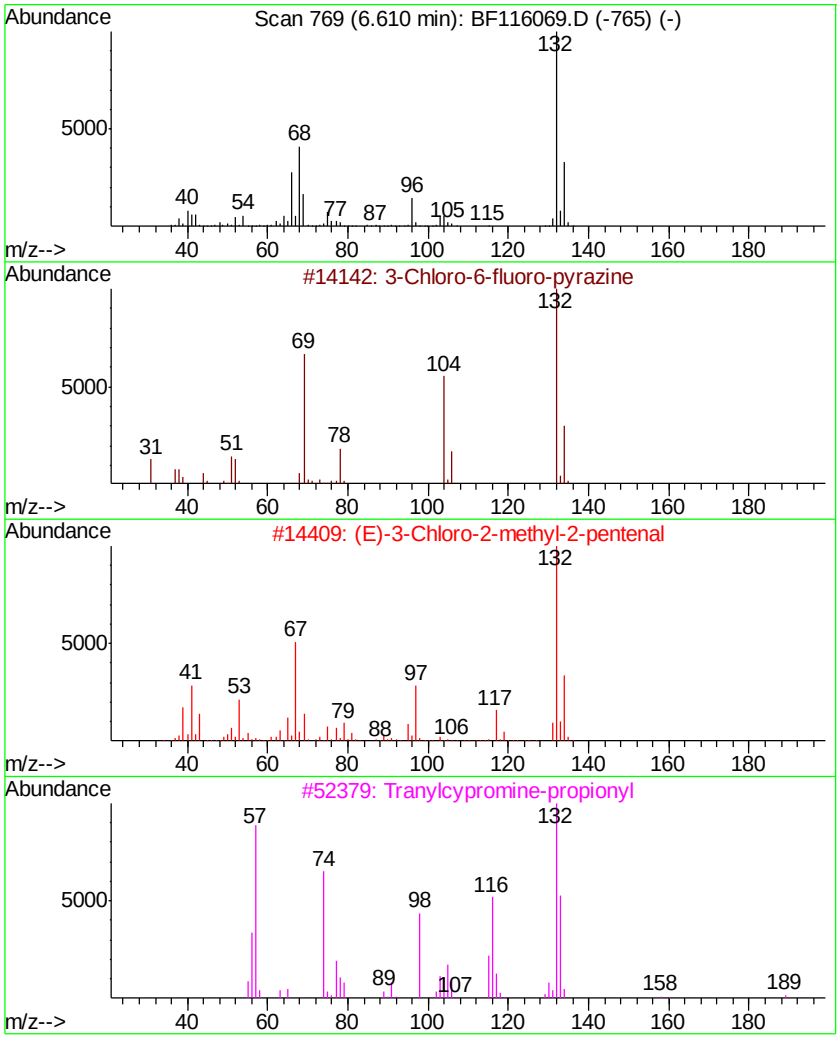
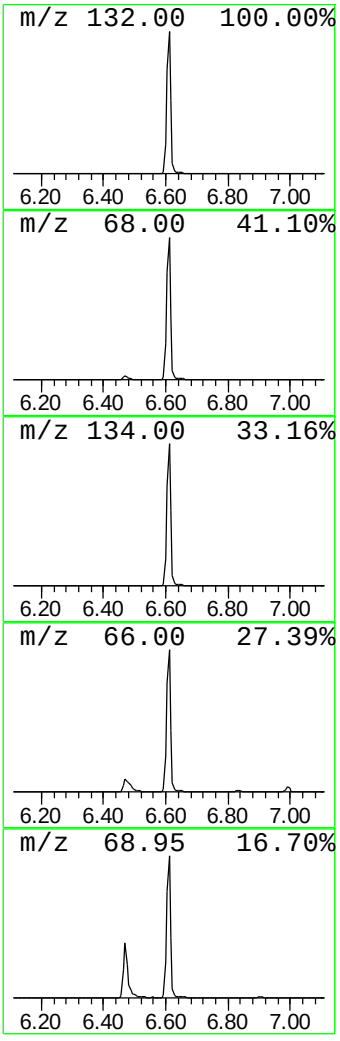
Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	70.87 ng	2770040	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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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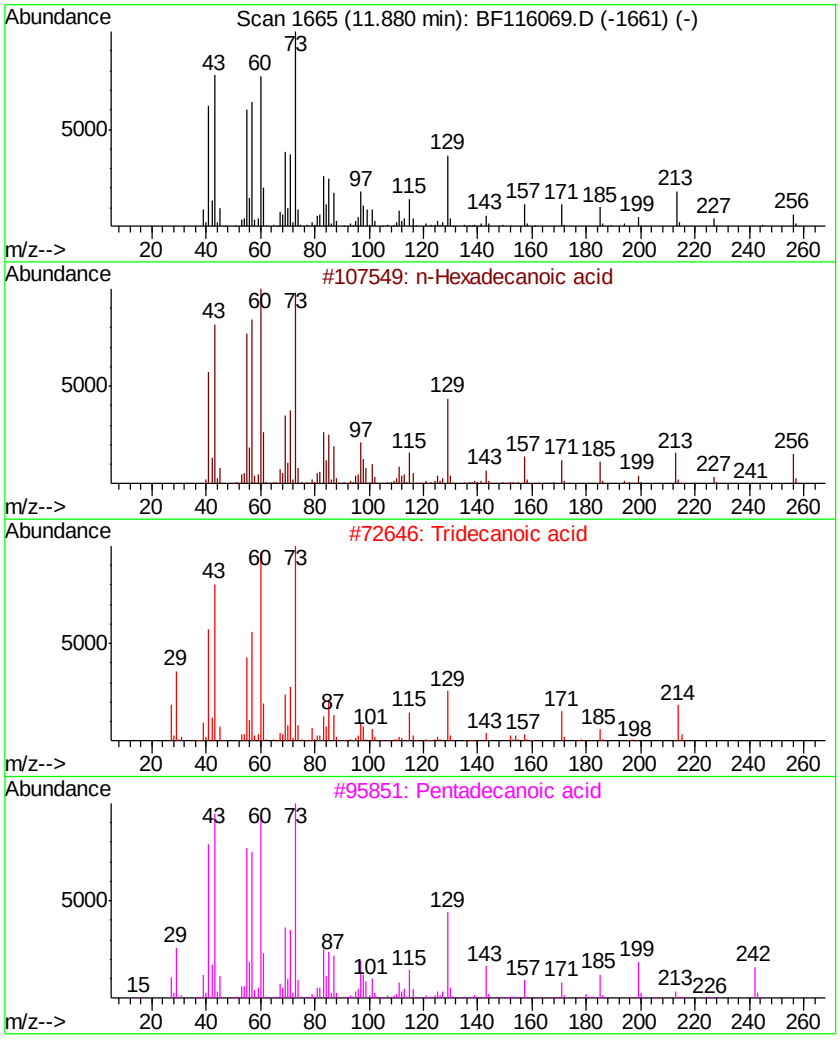
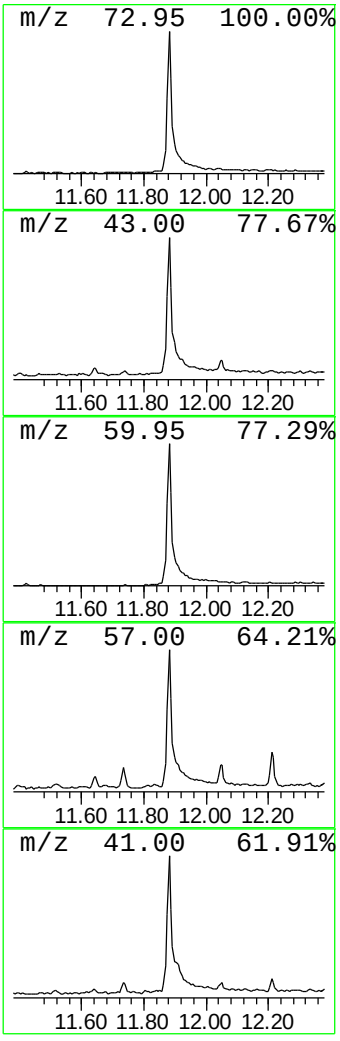
Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	7.02 ng	470003	Phenanthrene-d10	11.36

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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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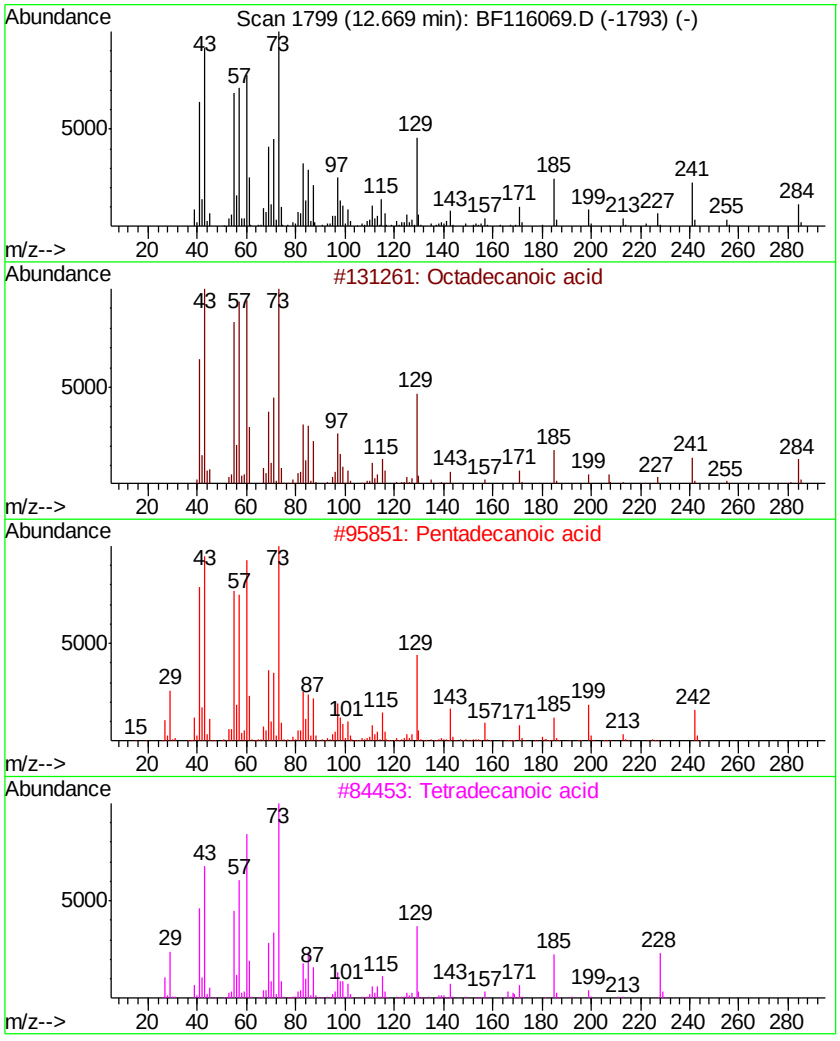
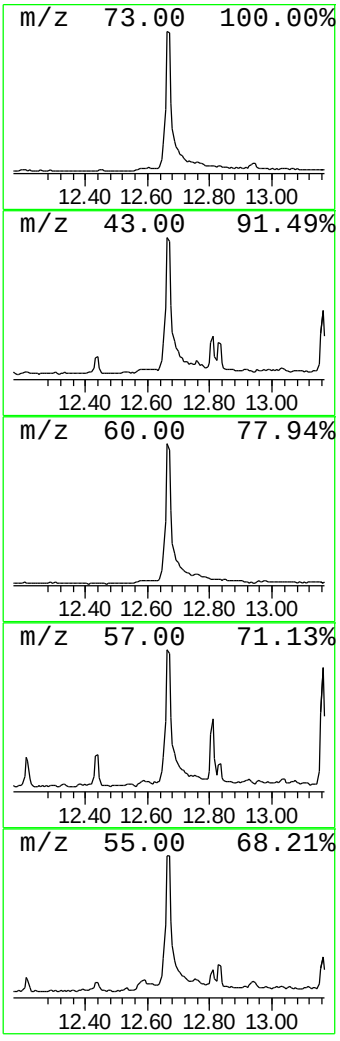
Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	10.89 ng	728880	Phenanthrene-d10	11.36

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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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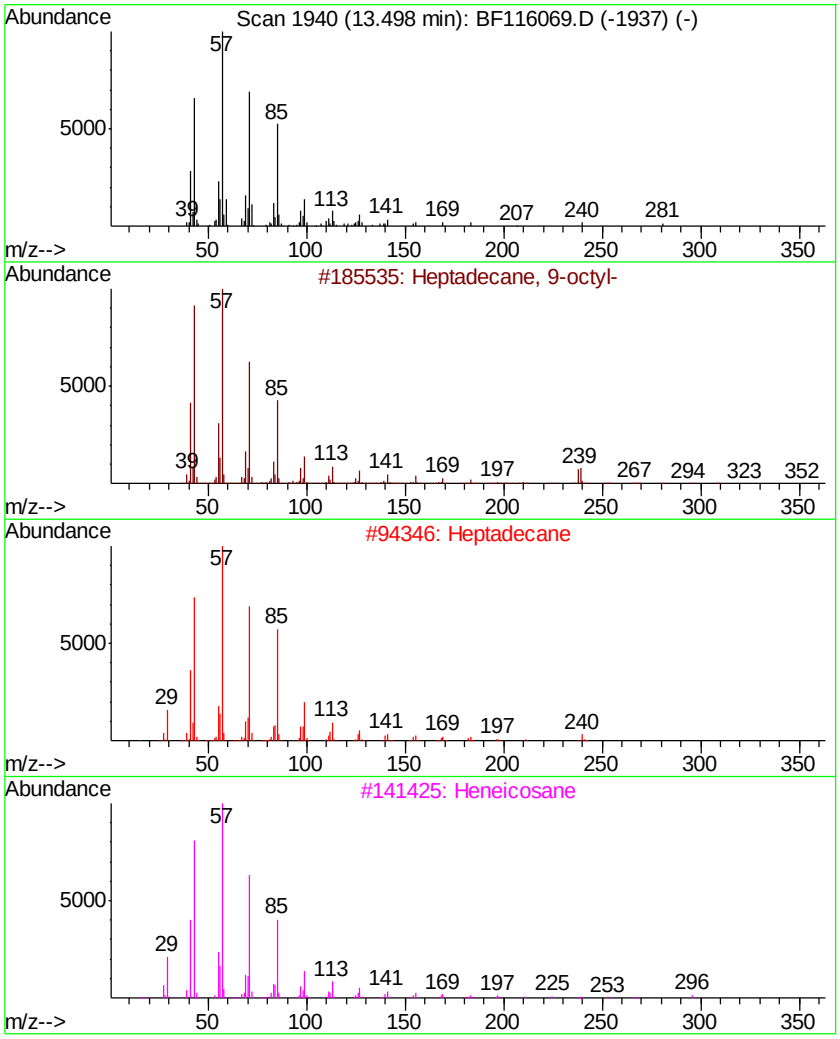
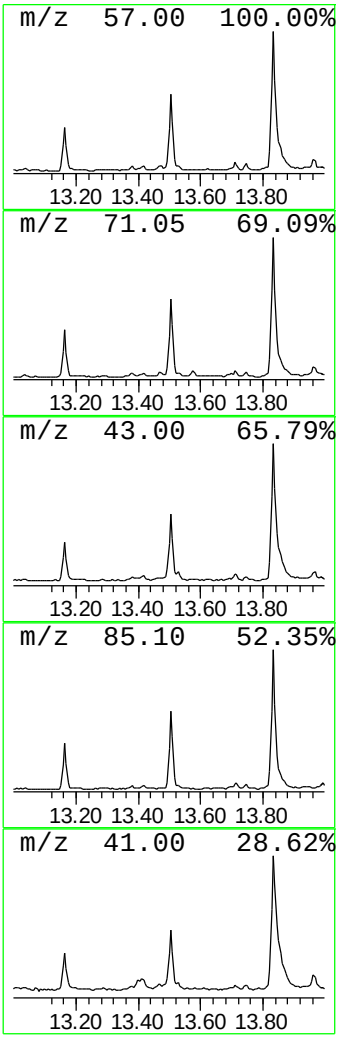
Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.76 ng	205200	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

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Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

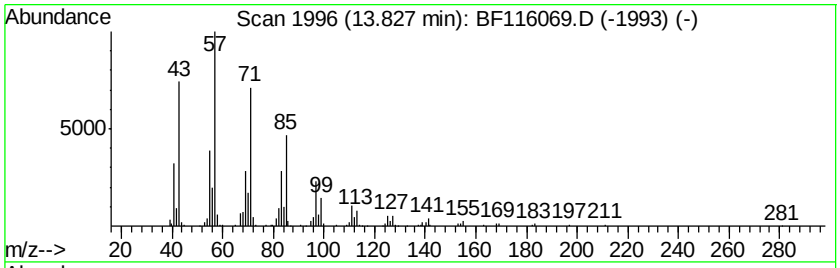
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

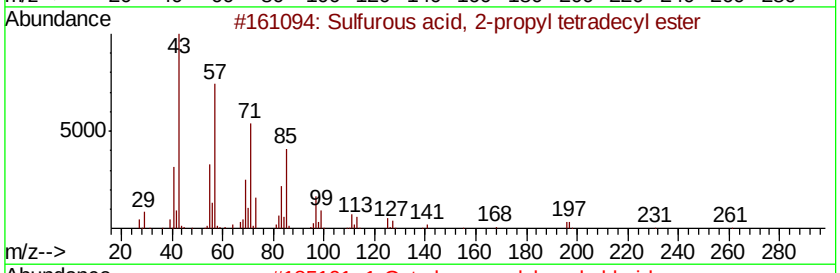
****

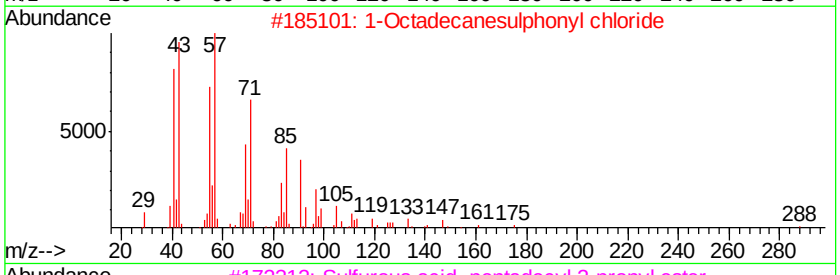
Peak Number 6 Sulfurous acid, 2-propyl te... Concentration Rank 3

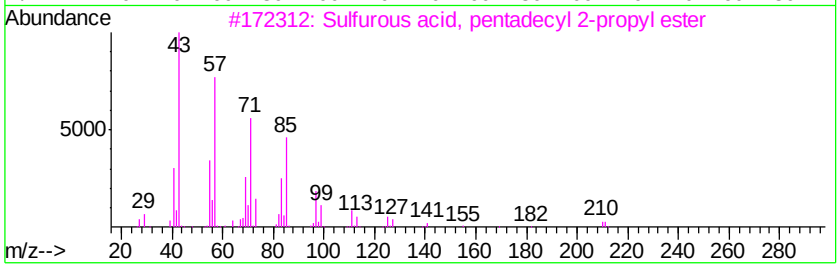
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	10.92 ng	812248	Chrysene-d12	14.00

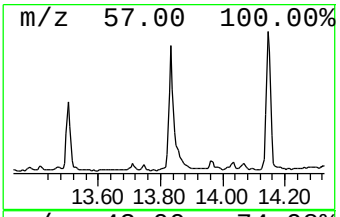
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	91
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
3	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
4	Nonadecane	268	C19H40	000629-92-5	68
5	Tetradecane	198	C14H30	000629-59-4	62

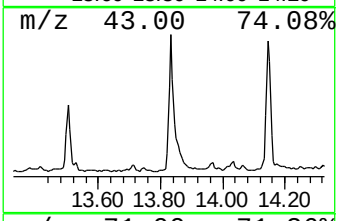


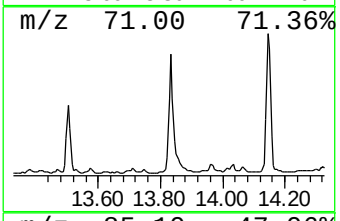


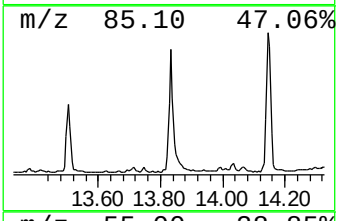


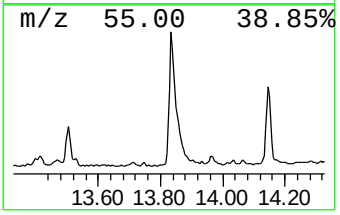












Library Search Compound Report

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ClientSampleId : COMP-BH-1-ELU-20190610

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

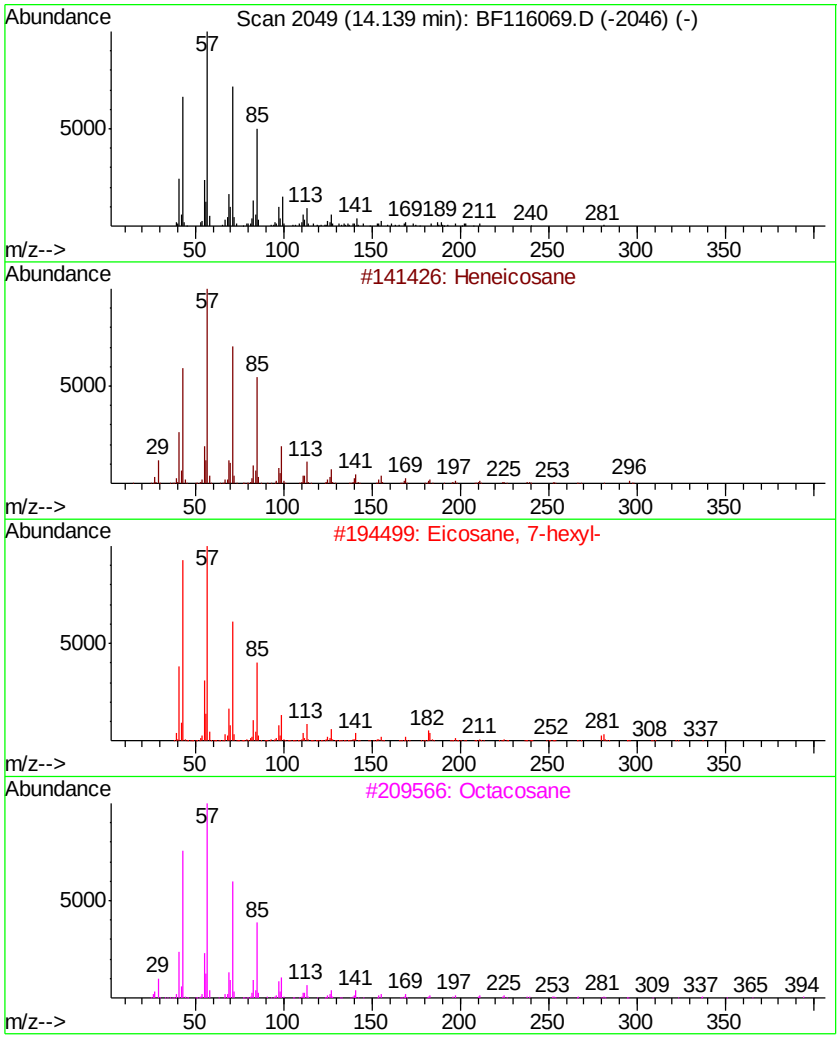
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

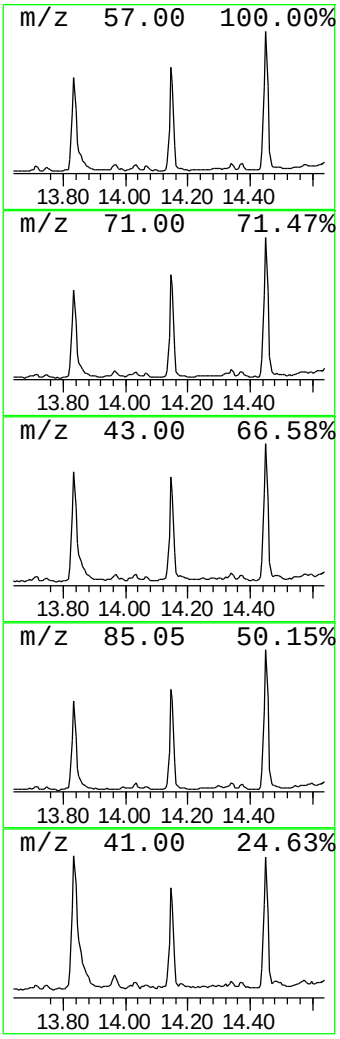
****

Peak Number 7 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	6.52 ng	484665	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexadecane	226	C16H34	000544-76-3	87
5	Octadecane	254	C18H38	000593-45-3	72





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Data File : BF116069.D
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Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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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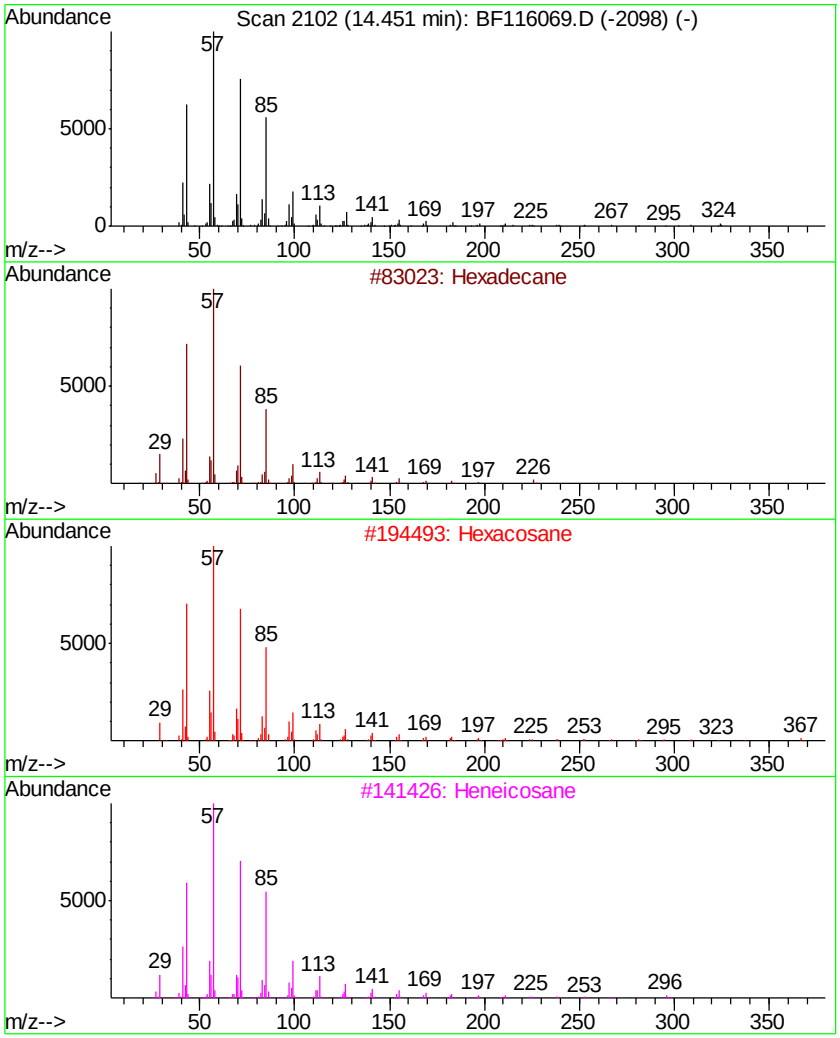
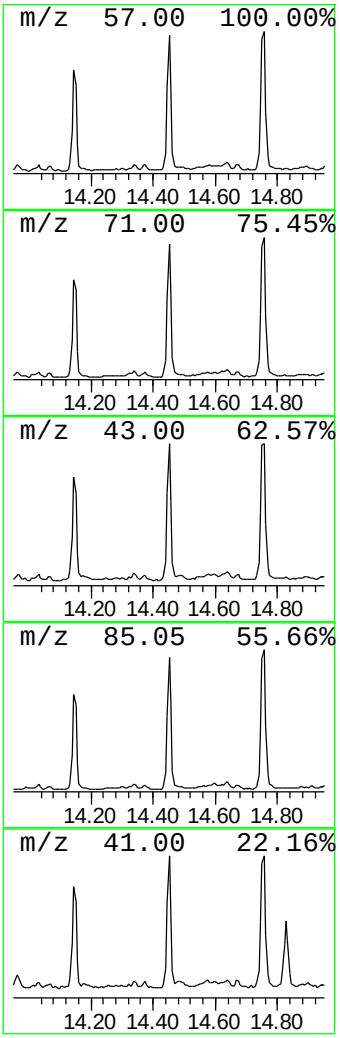
Peak Number 8 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	8.14 ng	605129	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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ClientSampleId : COMP-BH-1-ELU-20190610

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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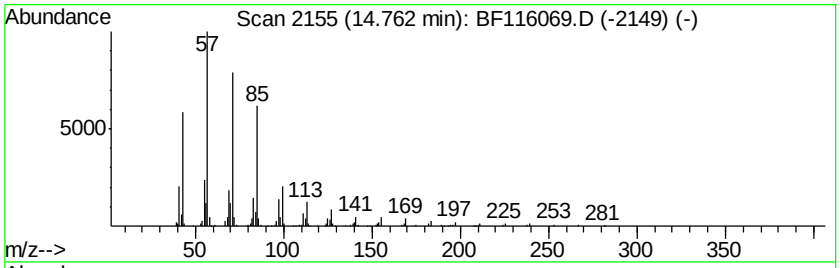
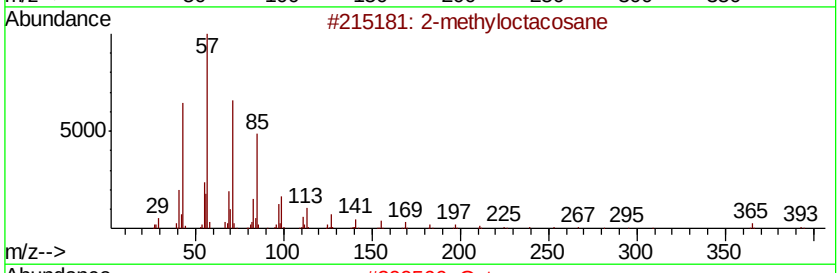
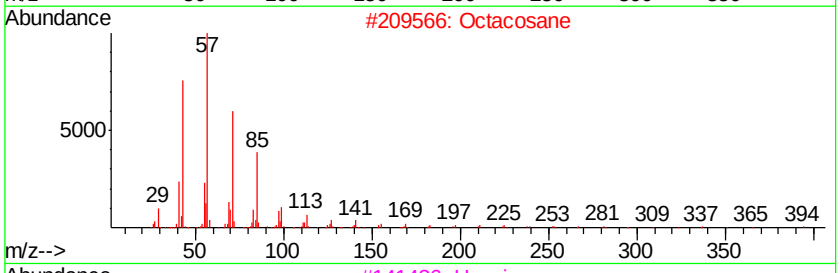
Peak Number 9 2-methyloctacosane Concentration Rank 7

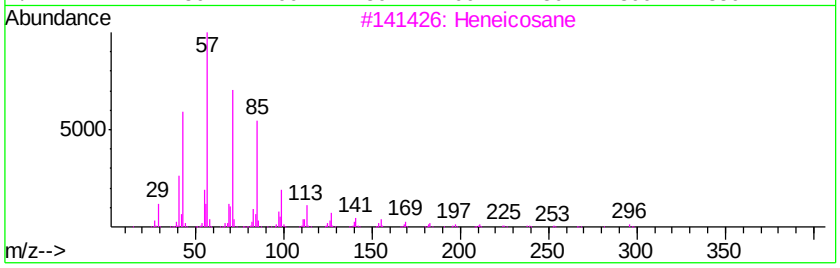
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	7.22 ng	746284	Perylene-d12	15.46

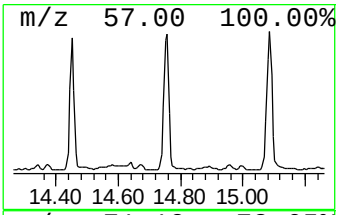
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heptadecane	240	C17H36	000629-78-7	91

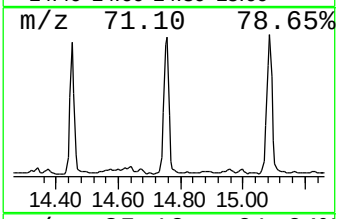


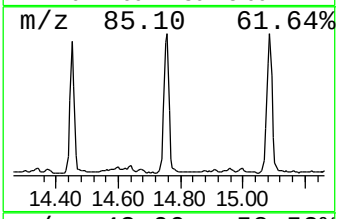


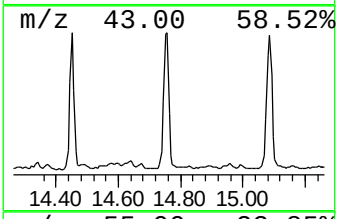


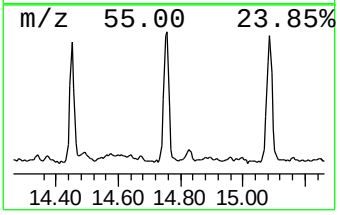












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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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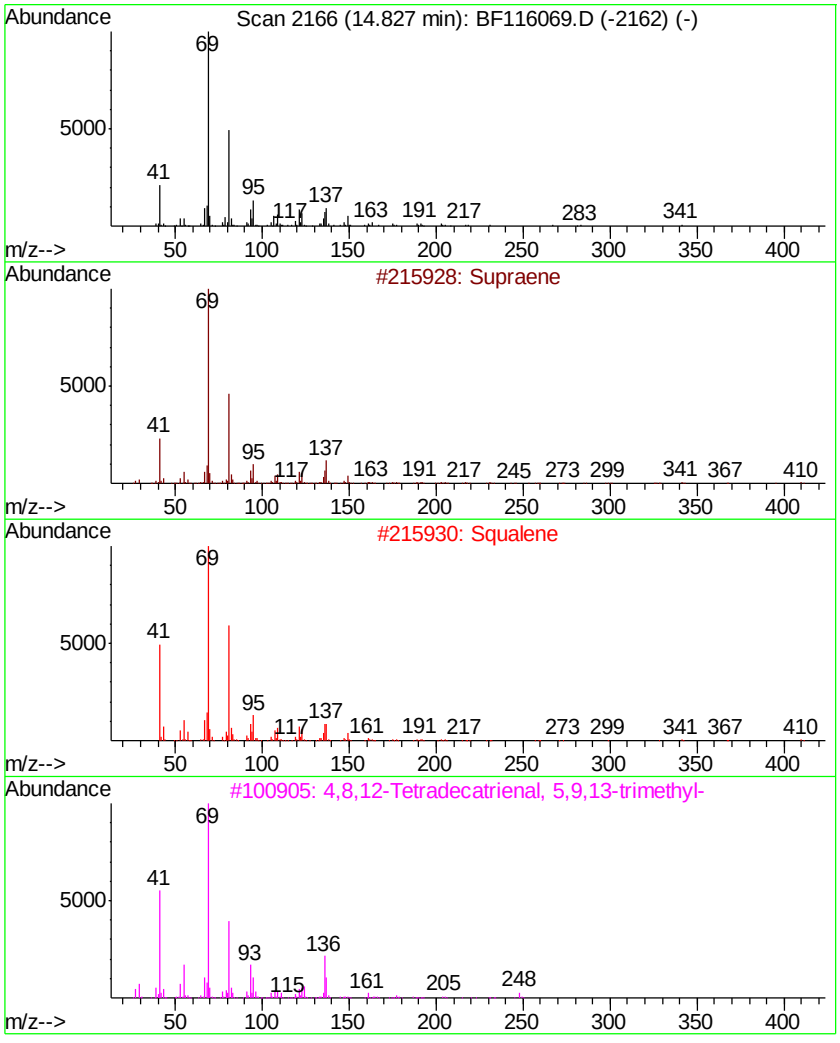
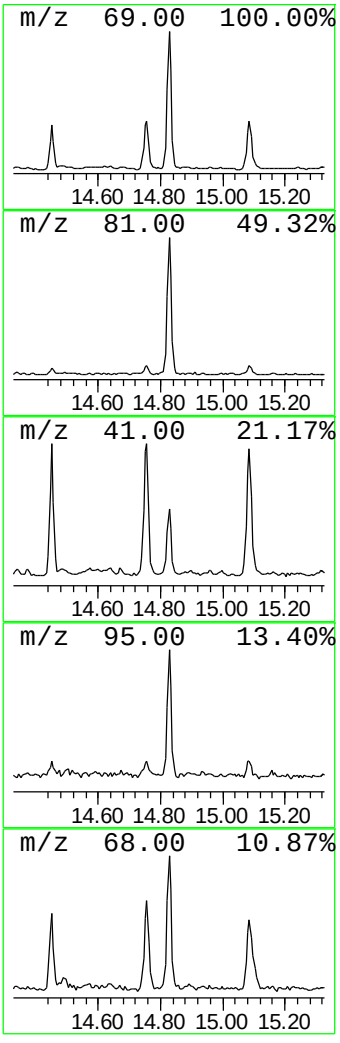
Peak Number 10 Supraene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.06 ng	212824	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	Farnesol isomer a	222	C15H26O	1000108-92-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080819\
Data File : BF116069.D
Acq On : 8 Aug 2019 15:19
Operator : HP/JU
Sample : K4148-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-1-ELU-20190610

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
unknown6.61	6.61	70.9	ng	2770040	1	6.83	781770	20.0
n-Hexadecanoic acid	11.88	7.0	ng	470003	4	11.36	1339150	20.0
Octadecanoic acid	12.67	10.9	ng	728880	4	11.36	1339150	20.0
Heptadecane, 9-oc...	13.50	2.8	ng	205200	5	14.00	1487110	20.0
Sulfurous acid, 2...	13.83	10.9	ng	812248	5	14.00	1487110	20.0
Heneicosane	14.14	6.5	ng	484665	5	14.00	1487110	20.0
Hexadecane	14.45	8.1	ng	605129	5	14.00	1487110	20.0
2-methyloctacosane	14.76	7.2	ng	746284	6	15.46	2067030	20.0
Supraene	14.83	2.1	ng	212824	6	15.46	2067030	20.0