LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 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-BF121918.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	2.193	12	18	33	rVB	334800	500075	10.77%	1.410%
2	5.104	507	513	520	rBV	115721	132719	2.86%	0.374%
3	5.522	580	584	598	rBV	1833070	1702463	36.68%	4.802%
4	6.528	751	755	766	rBV2	1254253	1185502	25.54%	3.344%
5	6.669	774	779	782	rBV	3625111	3246654	69.95%	9.157%
6	6.716	784	787	792	rVB	225977	186141	4.01%	0.525%
7	6.893	813	817	821	rBV	1220632	985709	21.24%	2.780%
8	7.051	840	844	847	rBV	3544893	3060015	65.93%	8.631%
9	7.451	907	912	915	rBV	2494666	2518646	54.26%	7.104%
10	7.657	943	947	950	rVB	80912	70214	1.51%	0.198%
11	8.175	1031	1035	1039	rBV	1486533	1255414	27.05%	3.541%
12	9.251	1213	1218	1221	rBV	5328957	4641659	100.00%	13.092%
13	9.363	1233	1237	1241	rBV2	123035	112302	2.42%	0.317%
14	9.639	1280	1284	1287	rBV	540624	414449	8.93%	1.169%
15	9.892	1324	1327	1330	rBV	51932	51227	1.10%	0.144%
16	9.933	1330	1334	1338	rVB	1519894	1378122	29.69%	3.887%
17	10.722	1463	1468	1471	rBV	3014003	2666154	57.44%	7.520%
18	11.075	1524	1528	1533	rBV	90572	94551	2.04%	0.267%
19	11.275	1554	1562	1567	rBV3	45187	61440	1.32%	0.173%
20	11.416	1582	1586	1590	rBV	1402249	1141455	24.59%	3.219%
21	11.863	1659	1662	1668	rBV2	91285	103749	2.24%	0.293%
22	11.945	1672	1676	1685	rBV2	407325	419593	9.04%	1.183%
23	13.004	1851	1856	1859	rBV	3259675	3151252	67.89%	8.888%
24	13.898	2004	2008	2018	rVB2	201285	275576	5.94%	0.777%
25	14.057	2032	2035	2039	rVB	1260997	1070047	23.05%	3.018%
26	14.216	2059	2062	2066	rBV	173725	153122	3.30%	0.432%
27	14.521	2111	2114	2118	rVB	273658	236750	5.10%	0.668%
28	14.680	2138	2141	2145	rBV	85678	84568	1.82%	0.239%
29	14.833	2164	2167	2172	rVB	335714	324416	6.99%	0.915%
30	14.916	2176	2181	2185	rVV	1809851	1982507	42.71%	5.592%
31	15.180	2222	2226	2230	rBV	315000	361575	7.79%	1.020%
32	15.545	2282	2288	2290	rBV	780873	1073054	23.12%	3.026%
33	16.010	2358	2367	2372	rBV	240748	411647	8.87%	1.161%
34	16.245	2405	2407	2418	rVB5	43735	100516	2.17%	0.283%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 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-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.445	2437	2441	2448	rVB9	64403	109761	2.36%	0.310%
36	16.527	2450	2455	2461	rBV	110365	192387	4.14%	0.543%

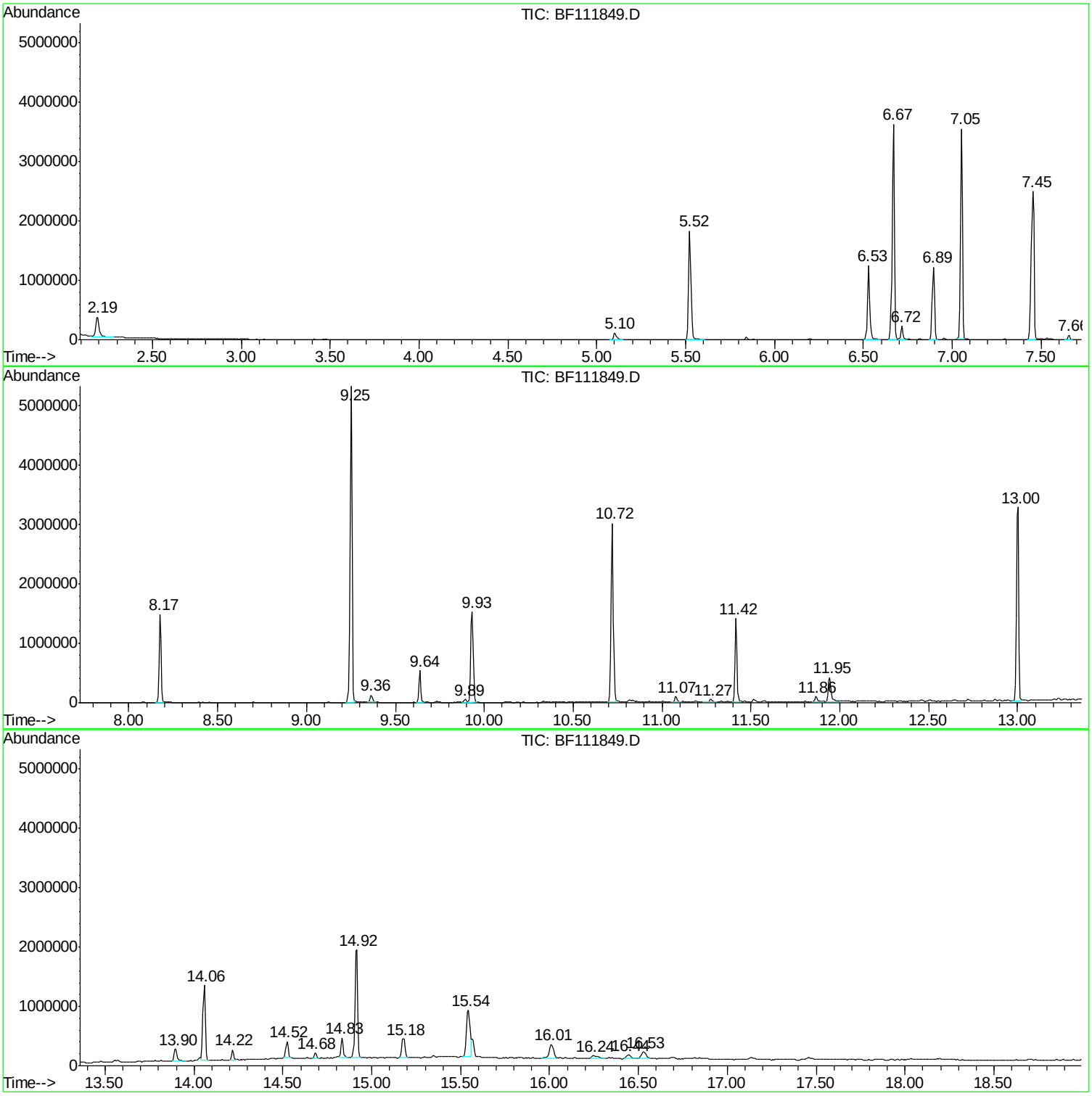
Sum of corrected areas: 35455431

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

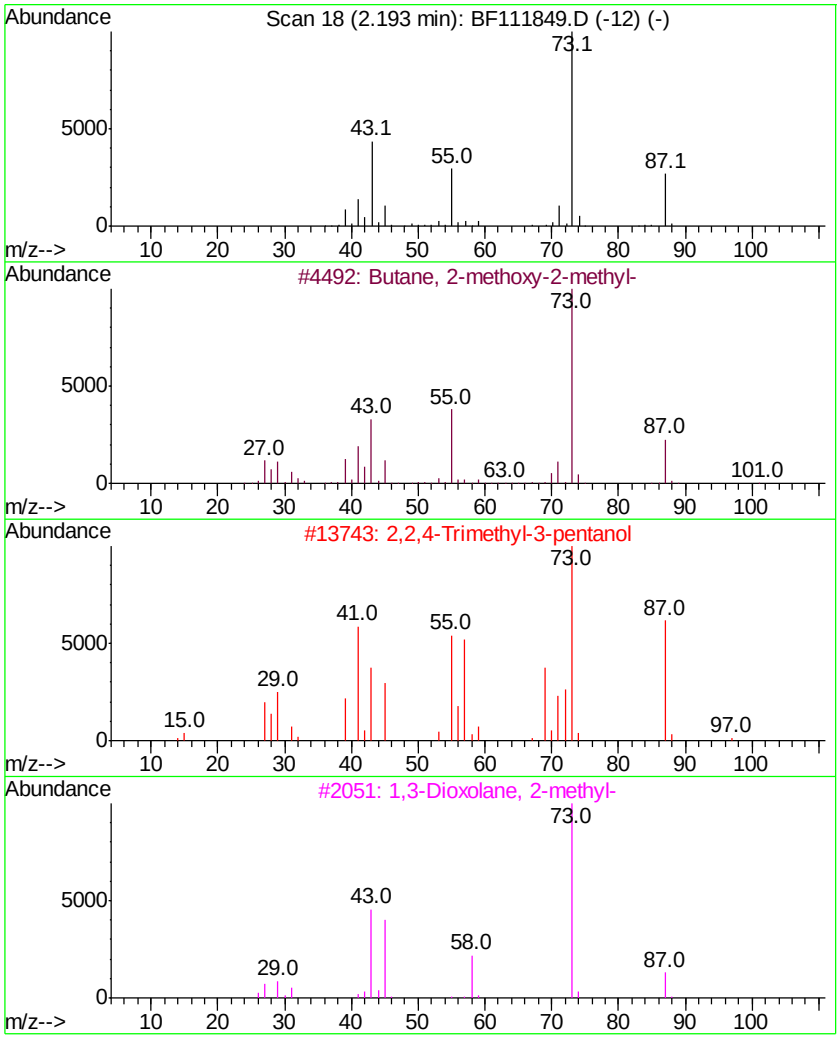
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

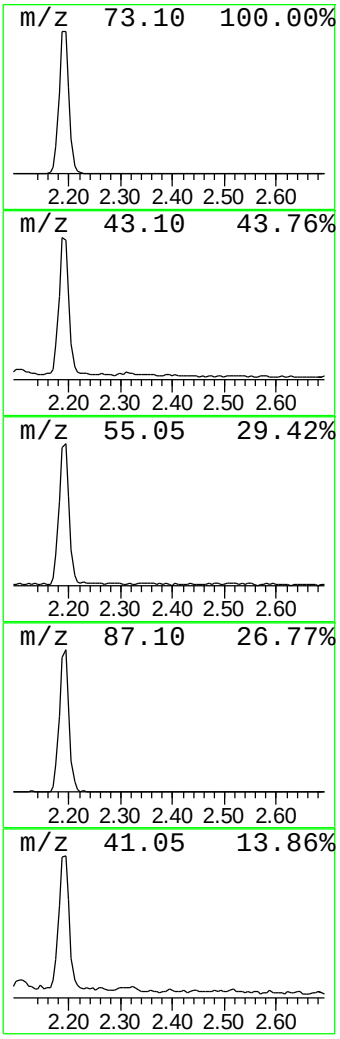
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	10.15 ng	500075	1,4-Dichlorobenzene-d4	6.89

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

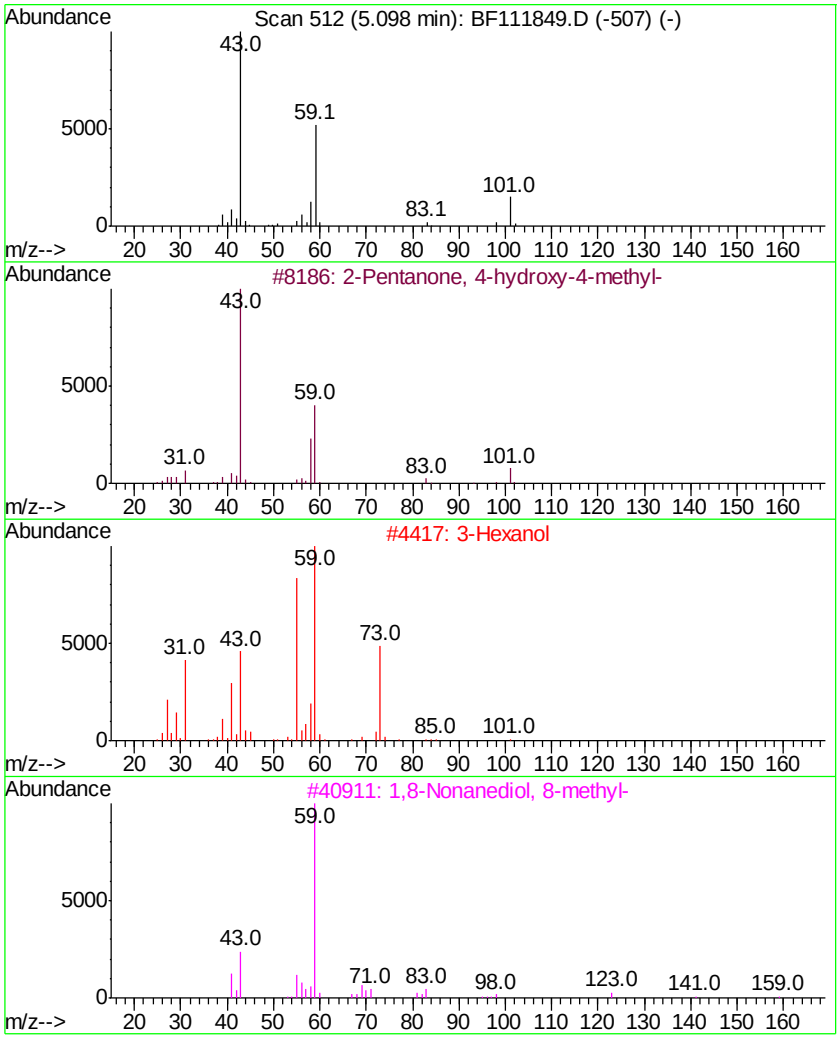
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

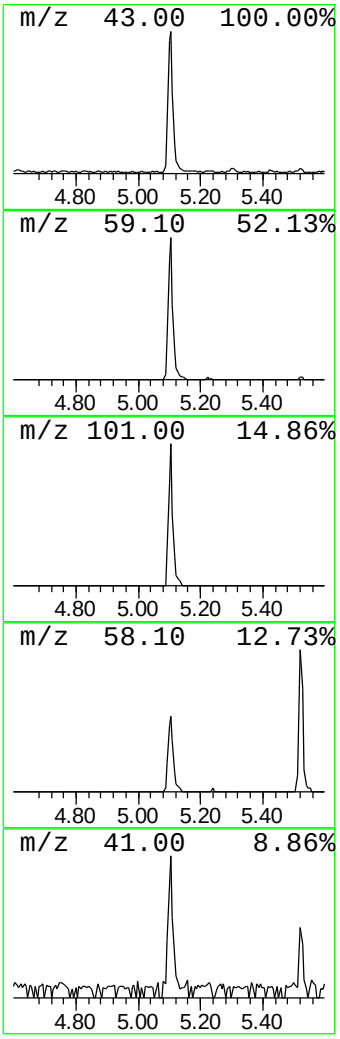
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.69 ng	132719	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	32
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

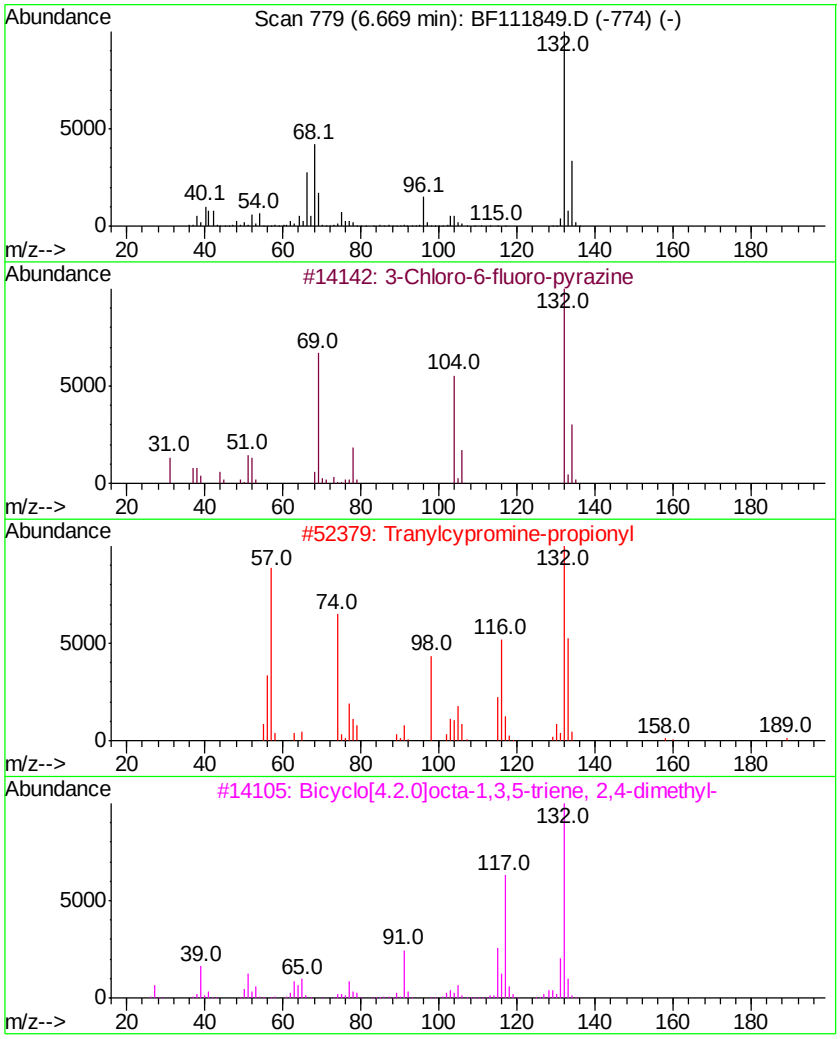
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

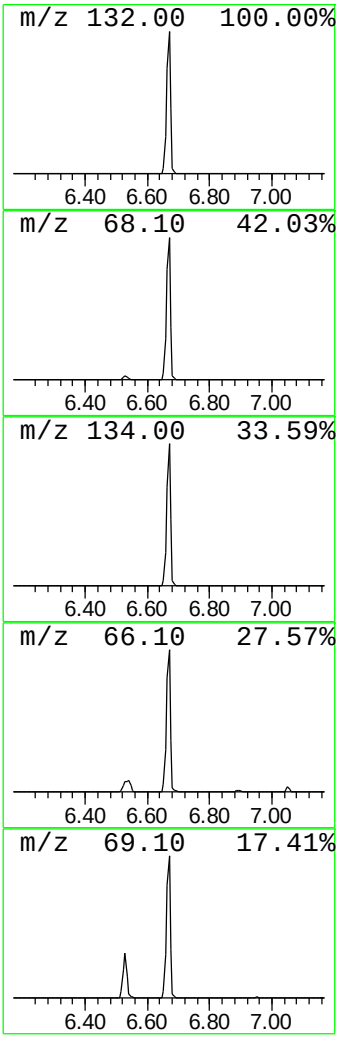
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	65.87 ng	3246650	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

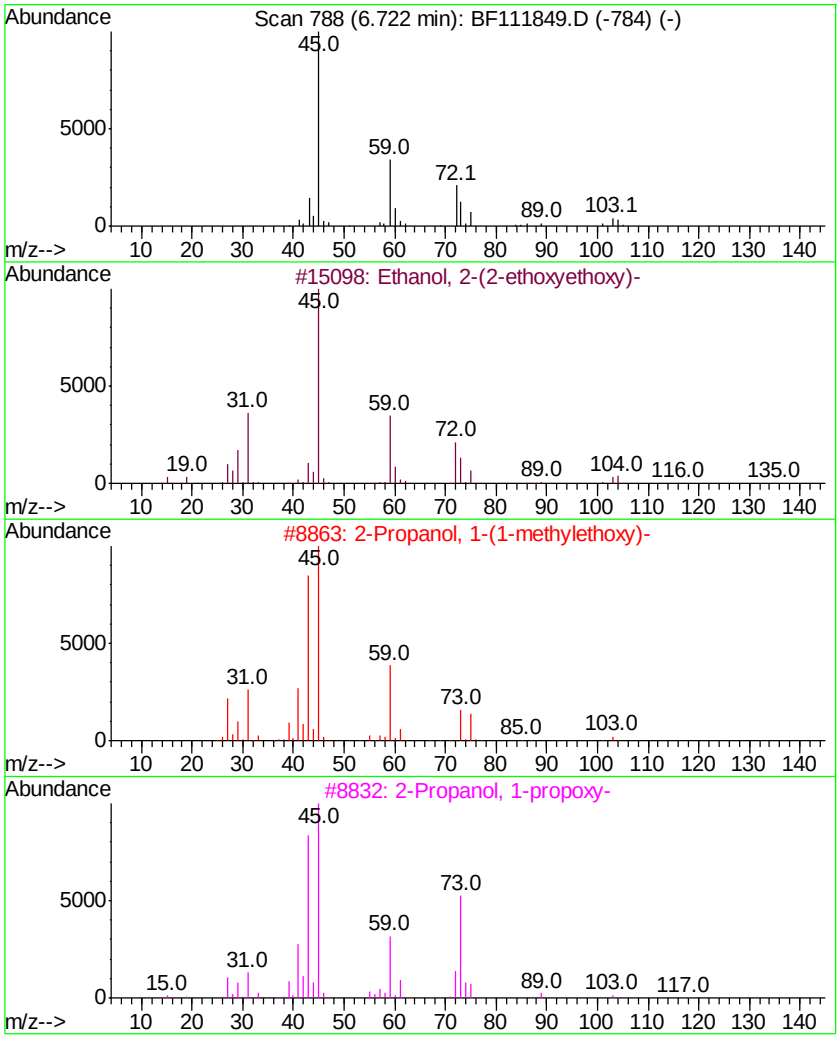
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

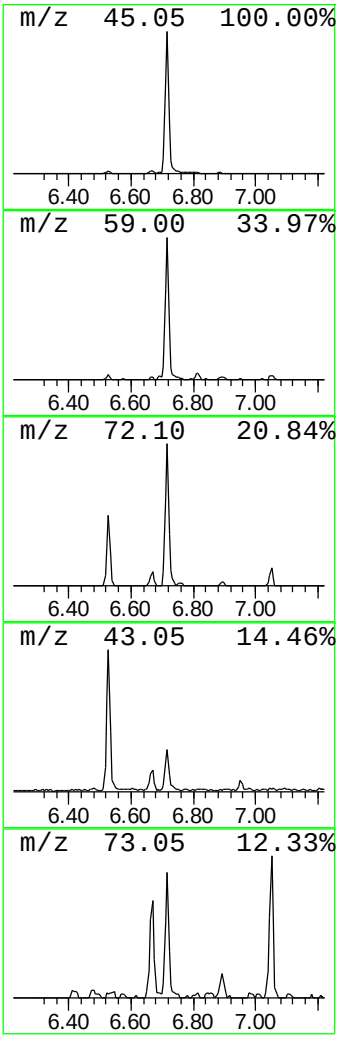
****

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	3.78 ng	186141	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37
5	Ethyl ether	74	C4H10O	000060-29-7	33





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

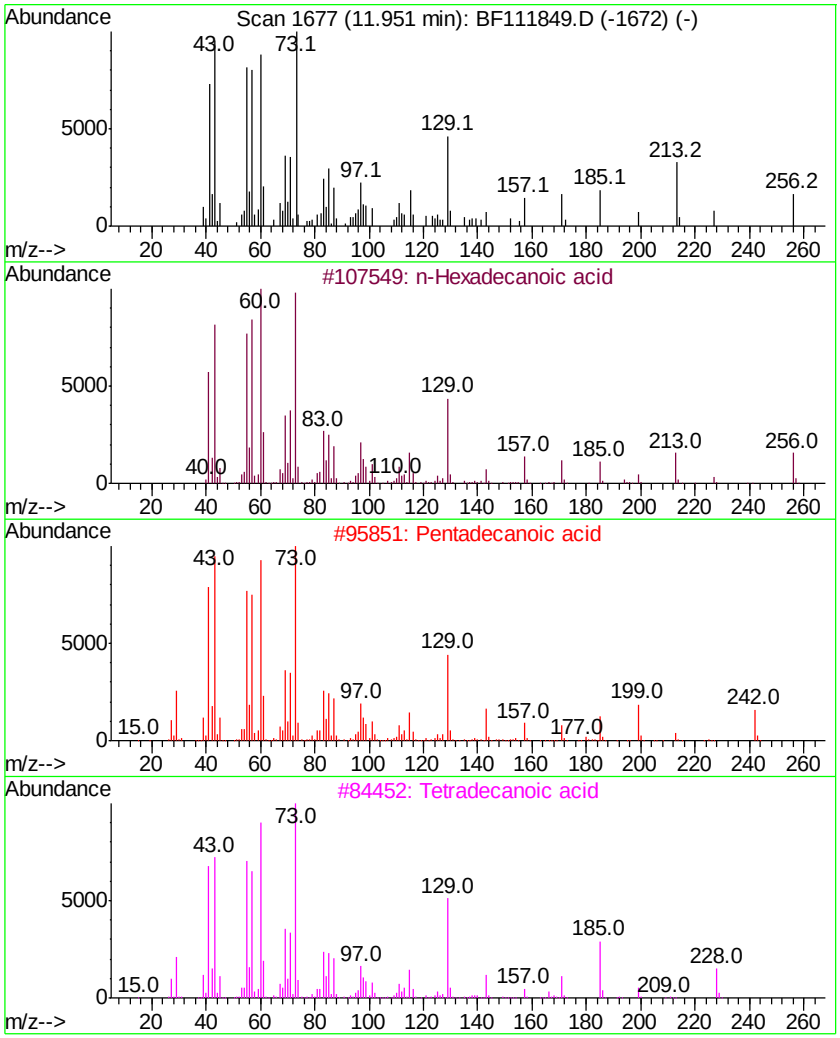
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

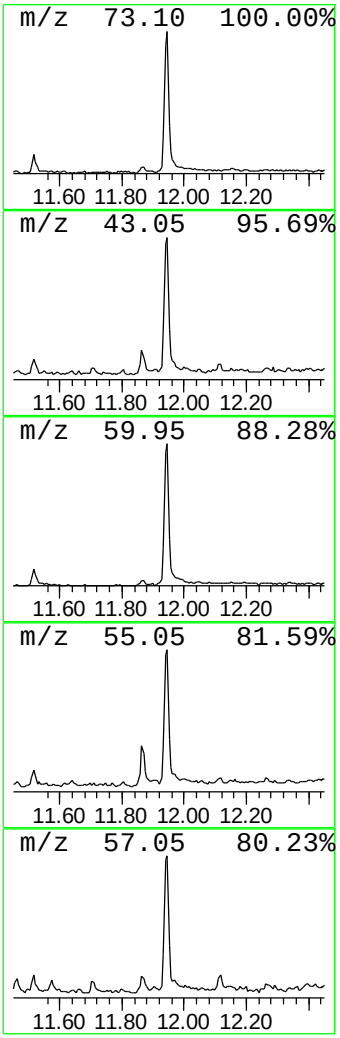
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	7.35 ng	419593	Phenanthrene-d10	11.42

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

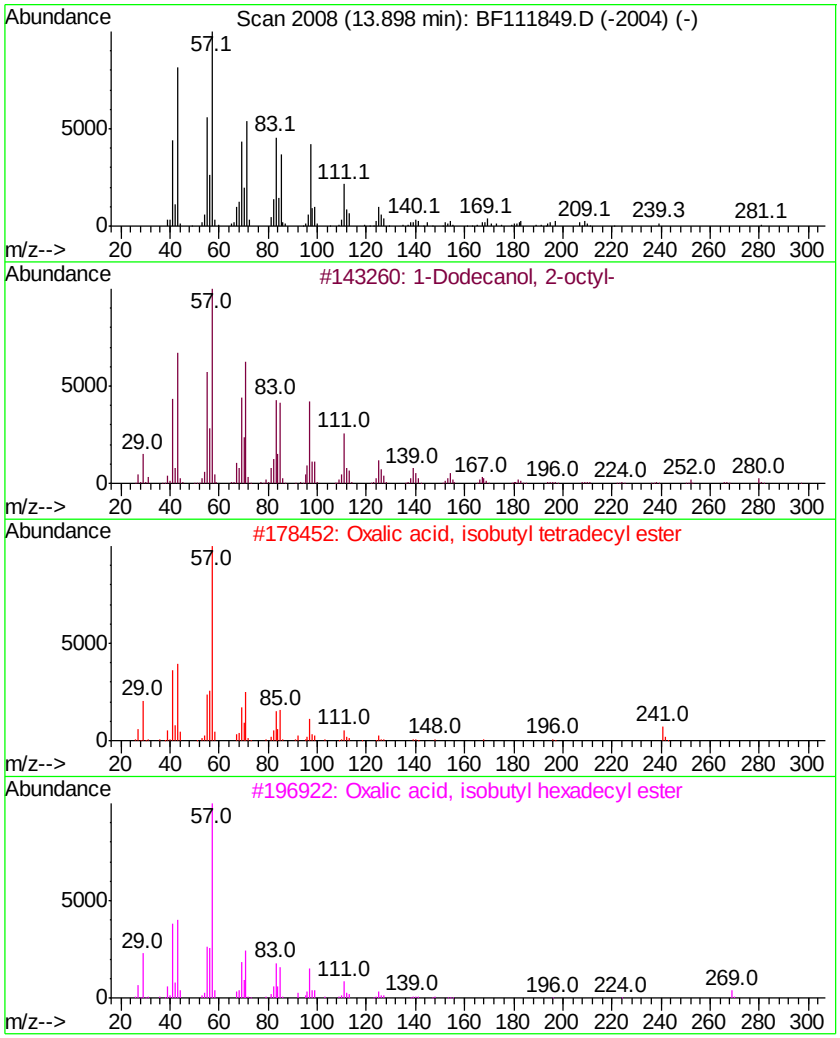
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

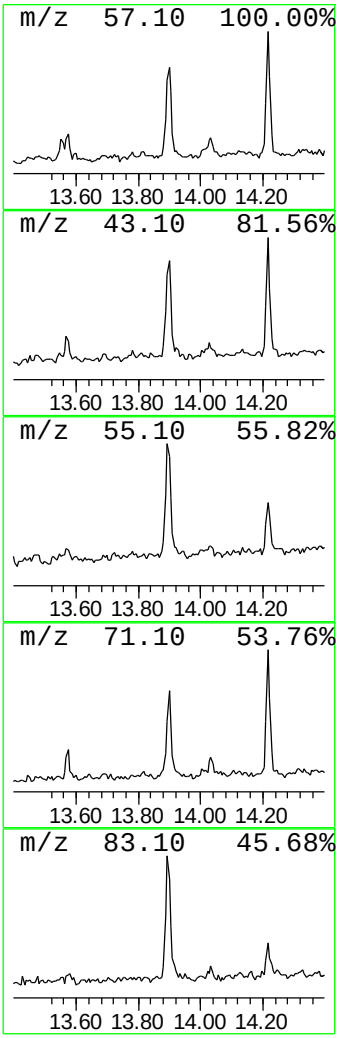
****

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	5.15 ng	275576	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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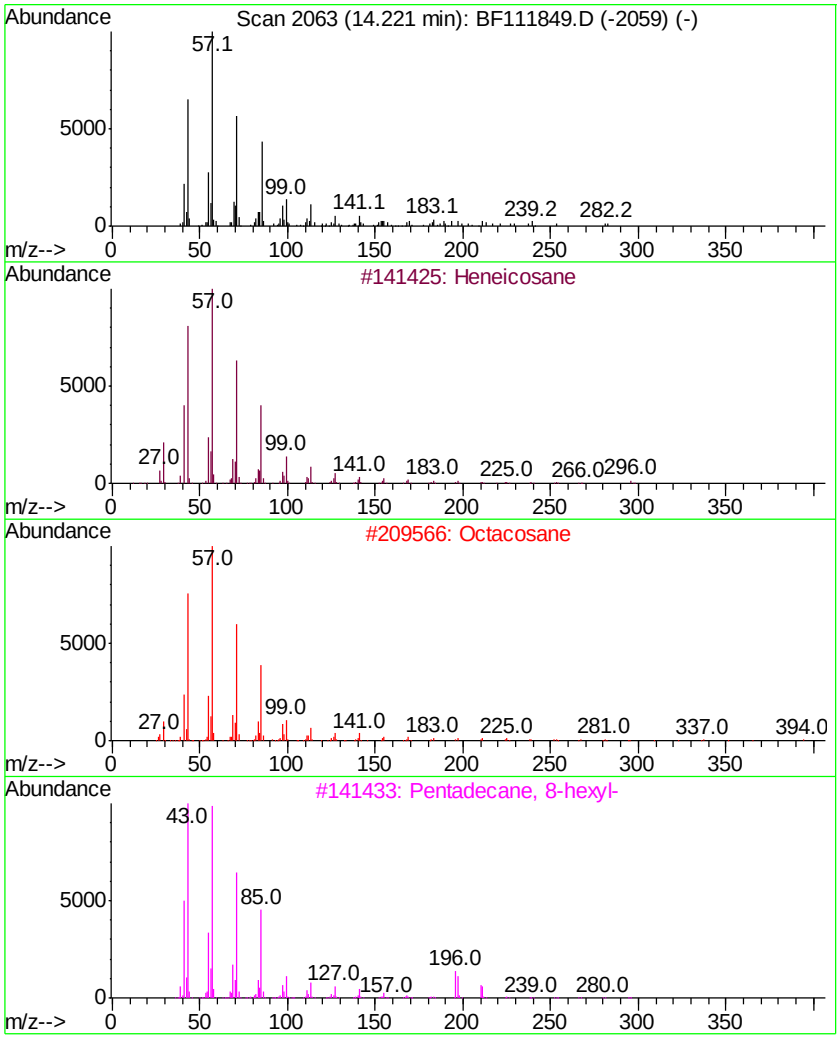
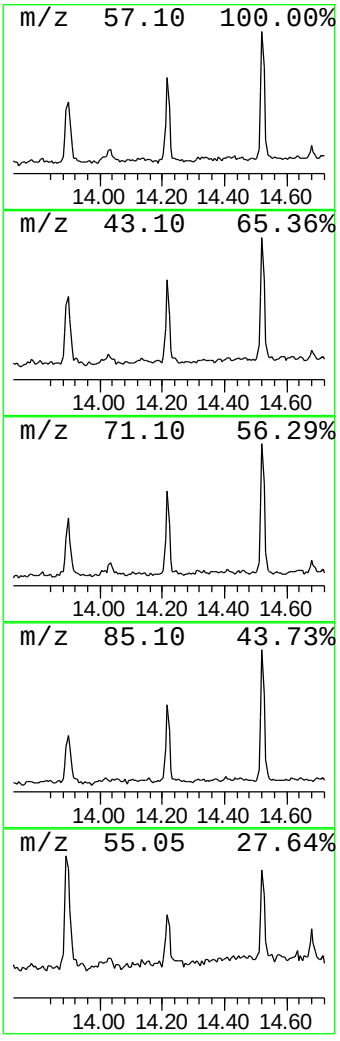
Peak Number 8 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	2.86 ng	153122	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
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Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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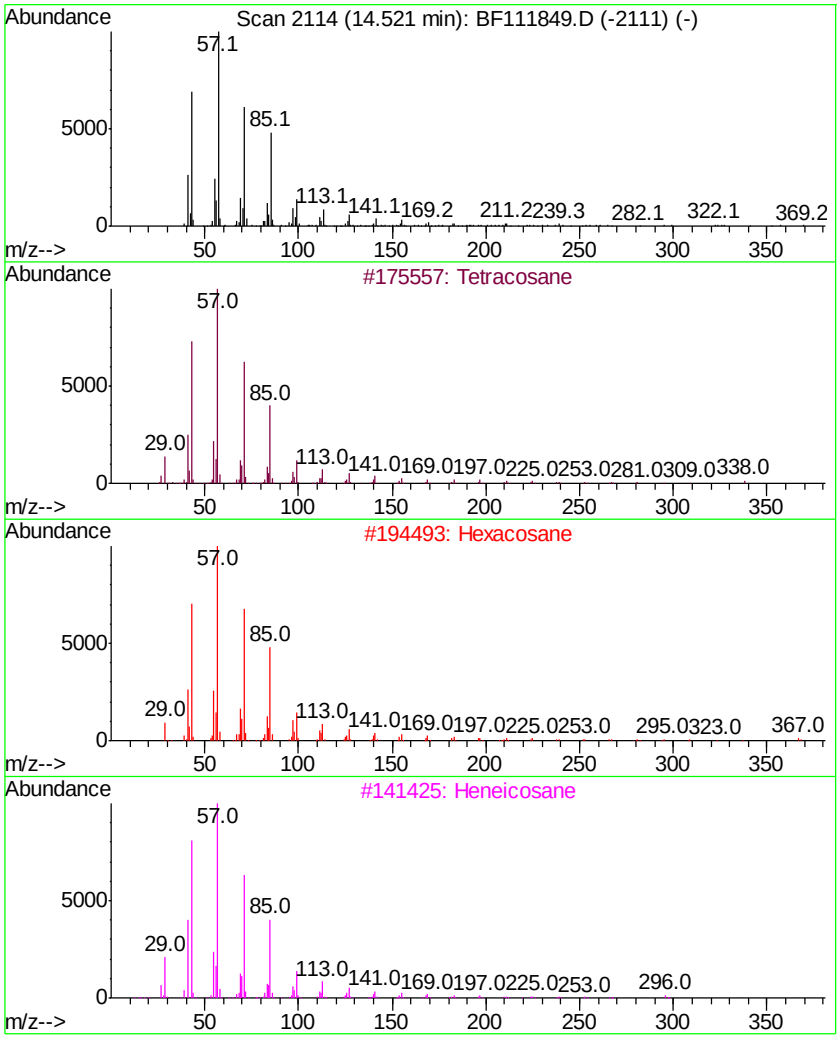
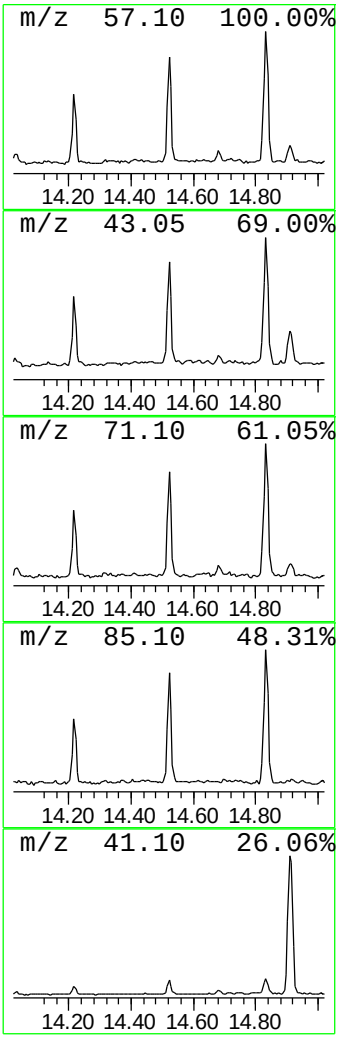
Peak Number 9 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	4.43 ng	236750	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octadecane	254	C18H38	000593-45-3	87
5	Nonadecane	268	C19H40	000629-92-5	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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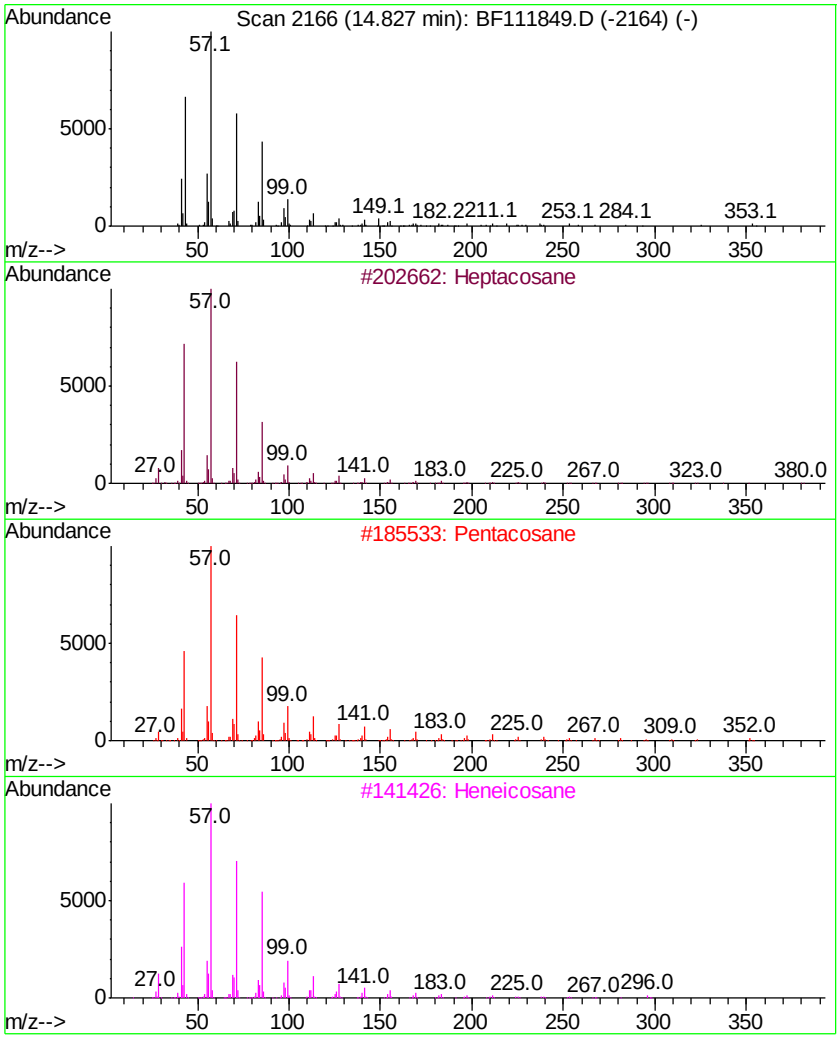
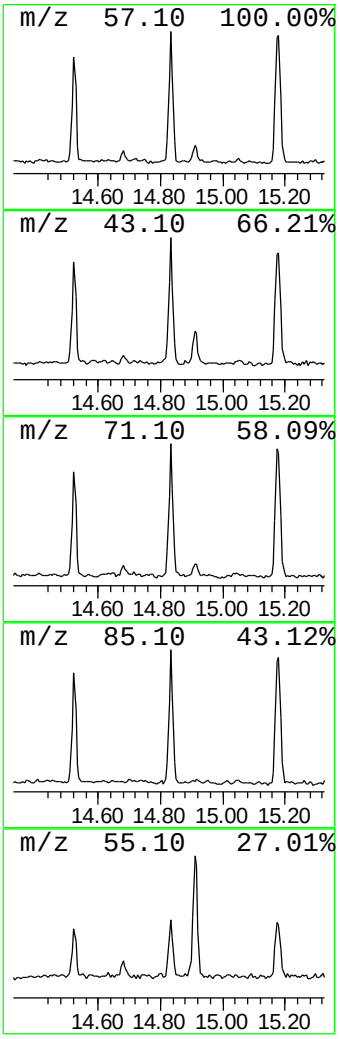
Peak Number 10 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	6.05 ng	324416	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heneicosane	296	C21H44	000629-94-7	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	83
5	Hexatriacontane	507	C36H74	000630-06-8	80





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Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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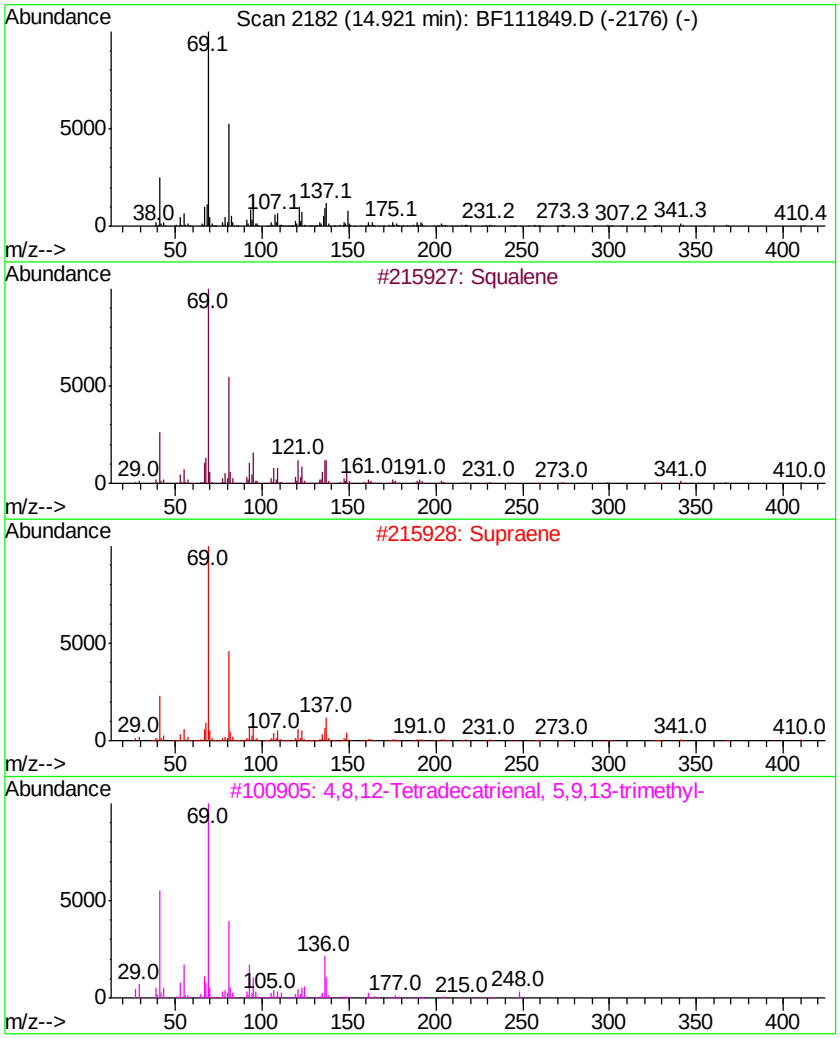
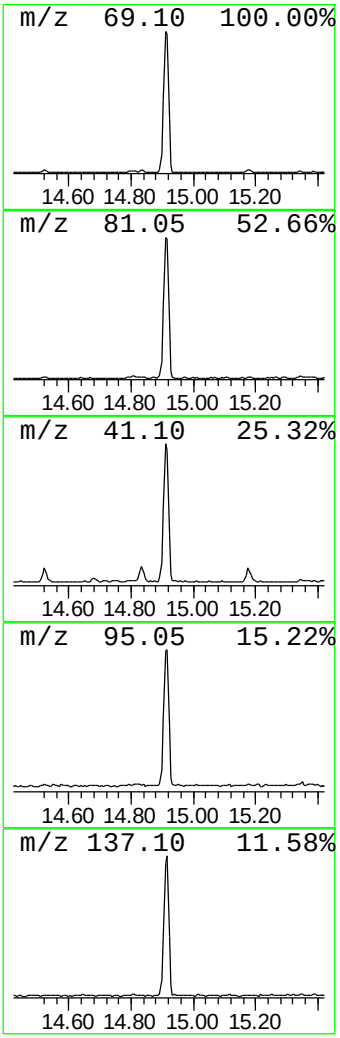
Peak Number 11 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	36.95 ng	1982510	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	95
2	Supraene	410	C30H50	007683-64-9	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





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Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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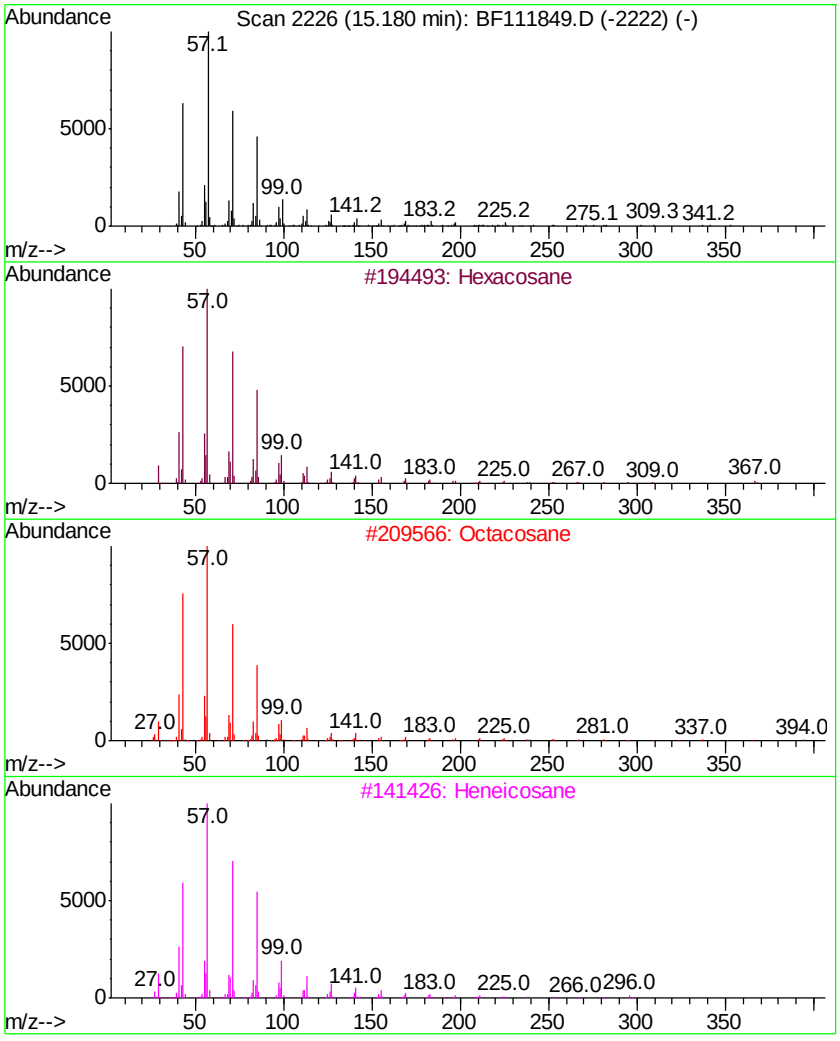
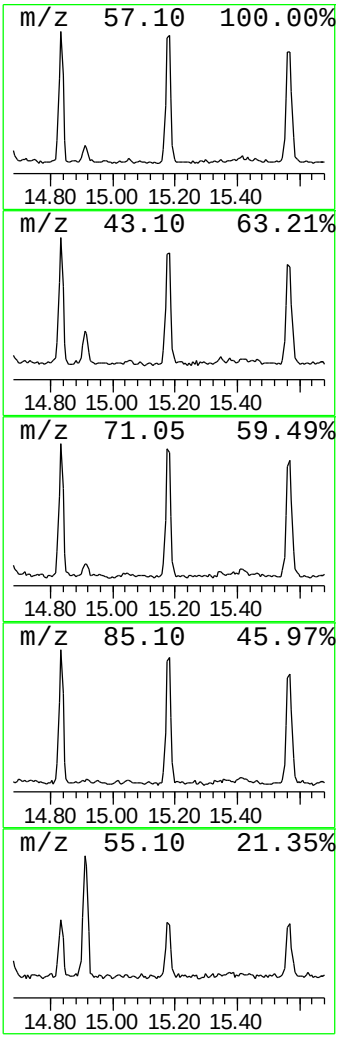
Peak Number 12 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	6.74 ng	361575	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Pentadecane, 8,8-diheptyl-	408	C29H60	055268-72-9	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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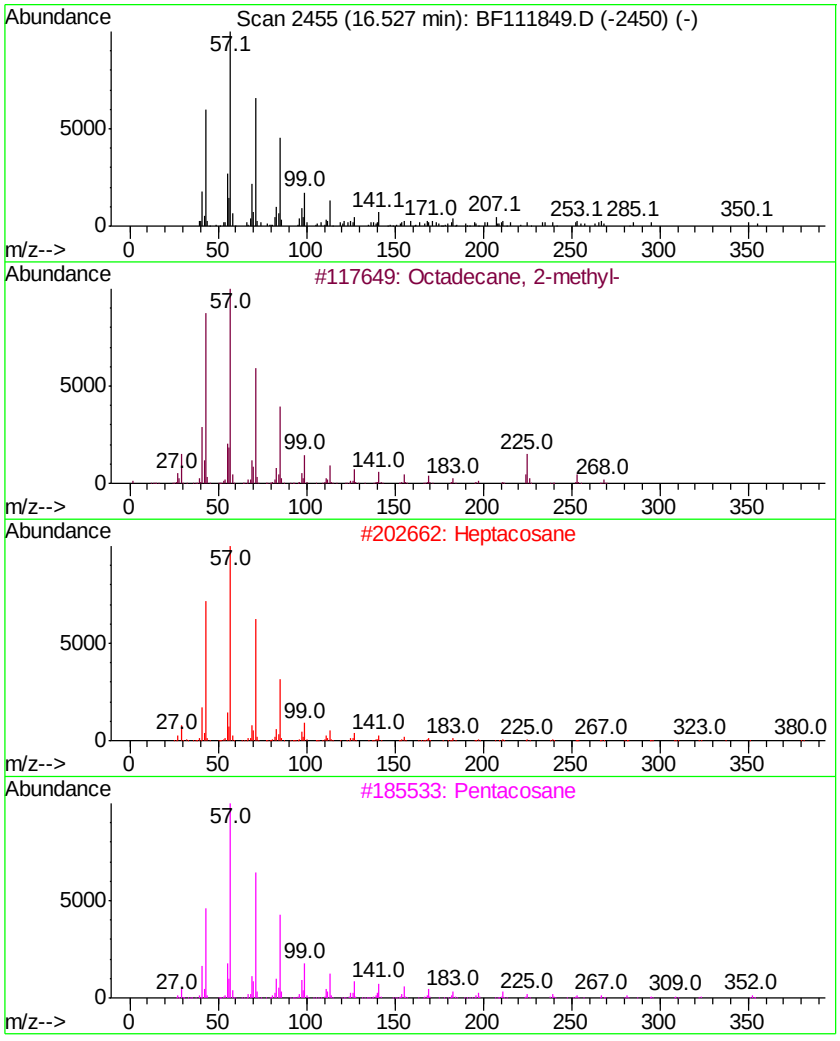
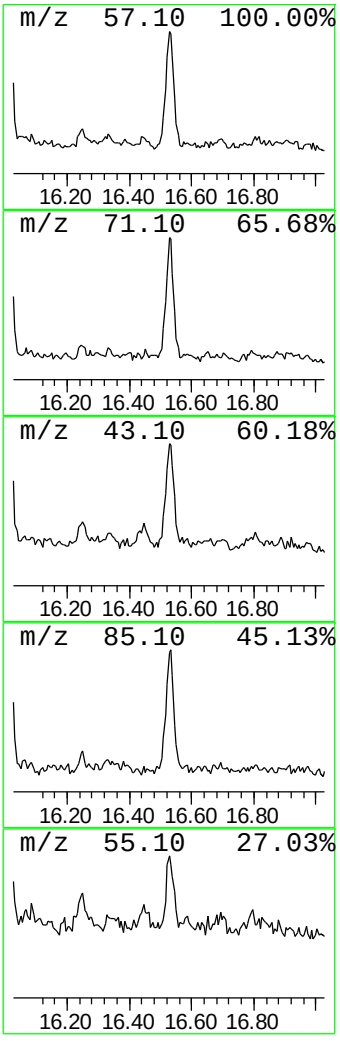
Peak Number 15 Octadecane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	3.59 ng	192387	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5	Octacosane	394	C28H58	000630-02-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010419\
Data File : BF111849.D
Acq On : 4 Jan 2019 17:19
Operator : JU/SJ
Sample : K1018-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	2.19	10.2	ng	500075	1	6.89	985709	20.0
2-Pentanone, 4-hy...	5.10	2.7	ng	132719	1	6.89	985709	20.0
unknown6.67	6.67	65.9	ng	3246650	1	6.89	985709	20.0
Ethanol, 2-(2-eth...	6.72	3.8	ng	186141	1	6.89	985709	20.0
n-Hexadecanoic acid	11.95	7.3	ng	419593	4	11.42	1141460	20.0
1-Dodecanol, 2-oc...	13.90	5.2	ng	275576	5	14.06	1070050	20.0
Heneicosane	14.22	2.9	ng	153122	5	14.06	1070050	20.0
Tetracosane	14.52	4.4	ng	236750	5	14.06	1070050	20.0
Heptacosane	14.83	6.0	ng	324416	6	15.54	1073050	20.0
Squalene	14.92	37.0	ng	1982510	6	15.54	1073050	20.0
Hexacosane	15.18	6.7	ng	361575	6	15.54	1073050	20.0
Octadecane, 2-met...	16.53	3.6	ng	192387	6	15.54	1073050	20.0