LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117709.D
Acq On : 7 Nov 2019 17:19
Operator : JU
Sample : K5723-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

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-BF110619.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	2.228	19	24	39	rVB	1046429	1487688	25.86%	2.394%
2	3.451	229	232	243	rBV	40279	82657	1.44%	0.133%
3	5.146	515	520	527	rVB	946943	1038598	18.05%	1.671%
4	5.545	583	588	591	rBV	4706378	4459597	77.51%	7.177%
5	6.545	753	758	763	rBV	4986366	4898660	85.14%	7.883%
6	6.698	780	784	787	rBV	5435134	4894451	85.06%	7.876%
7	6.934	820	824	827	rVB	2515163	1900039	33.02%	3.058%
8	7.092	847	851	854	rVB	4549979	3909372	67.94%	6.291%
9	7.492	914	919	922	rBV	3381923	2951133	51.29%	4.749%
10	8.222	1037	1043	1046	rBV	2811343	2533912	44.04%	4.078%
11	9.298	1221	1226	1229	rBV	6630847	5753780	100.00%	9.259%
12	9.686	1289	1292	1297	rVB	950626	734639	12.77%	1.182%
13	9.980	1338	1342	1345	rVB	3540743	2839434	49.35%	4.569%
14	10.769	1471	1476	1479	rBV	3942332	3470975	60.33%	5.586%
15	10.869	1487	1493	1495	rBV	90577	91302	1.59%	0.147%
16	10.898	1495	1498	1502	rVB3	63224	77843	1.35%	0.125%
17	11.469	1591	1595	1598	rBV	3441922	2912126	50.61%	4.686%
18	11.492	1598	1599	1602	rVV	215428	121625	2.11%	0.196%
19	11.539	1602	1607	1610	rVB3	92839	108220	1.88%	0.174%
20	11.692	1629	1633	1636	rBV	138949	120454	2.09%	0.194%
21	11.992	1677	1684	1696	rBV2	838401	1042063	18.11%	1.677%
22	12.251	1725	1728	1730	rBV	87476	72588	1.26%	0.117%
23	12.522	1770	1774	1777	rBV3	61314	66678	1.16%	0.107%
24	12.563	1777	1781	1786	rBV2	85547	106332	1.85%	0.171%
25	12.686	1798	1802	1808	rBV	480915	470182	8.17%	0.757%
26	12.780	1815	1818	1822	rBV	283215	279850	4.86%	0.450%
27	12.916	1836	1841	1843	rBV	411593	342173	5.95%	0.551%
28	13.063	1861	1866	1869	rBV	6233225	5513552	95.82%	8.873%
29	13.345	1910	1914	1917	rBV2	58656	63795	1.11%	0.103%
30	13.639	1958	1964	1972	rVB2	80261	117323	2.04%	0.189%
31	13.751	1978	1983	1987	rBV	60739	77287	1.34%	0.124%
32	13.957	2015	2018	2025	rBV	557047	604722	10.51%	0.973%
33	14.116	2040	2045	2048	rBV	2496973	2417636	42.02%	3.891%
34	14.139	2048	2049	2057	rVB	199802	184135	3.20%	0.296%

LSC Area Percent Report

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Operator : JU
Sample : K5723-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

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-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.286	2070	2074	2079	rVB	169426	173683	3.02%	0.279%
36	14.592	2121	2126	2130	rBV	240786	236644	4.11%	0.381%
37	14.910	2176	2180	2190	rBV	219758	262955	4.57%	0.423%
38	14.992	2190	2194	2205	rVB	1307679	1329375	23.10%	2.139%
39	15.174	2221	2225	2229	rBV	191871	304883	5.30%	0.491%
40	15.268	2237	2241	2250	rVB2	212431	314884	5.47%	0.507%
41	15.492	2275	2279	2285	rVB	112646	149128	2.59%	0.240%
42	15.557	2286	2290	2295	rVB	130787	175601	3.05%	0.283%
43	15.627	2296	2302	2306	rBV	1913963	2333201	40.55%	3.755%
44	15.668	2306	2309	2318	rVB2	193468	283473	4.93%	0.456%
45	16.133	2383	2388	2392	rBV3	129600	213058	3.70%	0.343%
46	16.180	2393	2396	2406	rVB7	55825	121073	2.10%	0.195%
47	16.557	2456	2460	2469	rVB9	57243	109426	1.90%	0.176%
48	16.668	2474	2479	2484	rBV4	63051	121952	2.12%	0.196%
49	17.145	2555	2560	2570	rVB3	71004	160455	2.79%	0.258%
50	17.609	2634	2639	2648	rBV2	54501	106056	1.84%	0.171%

Sum of corrected areas: 62140668

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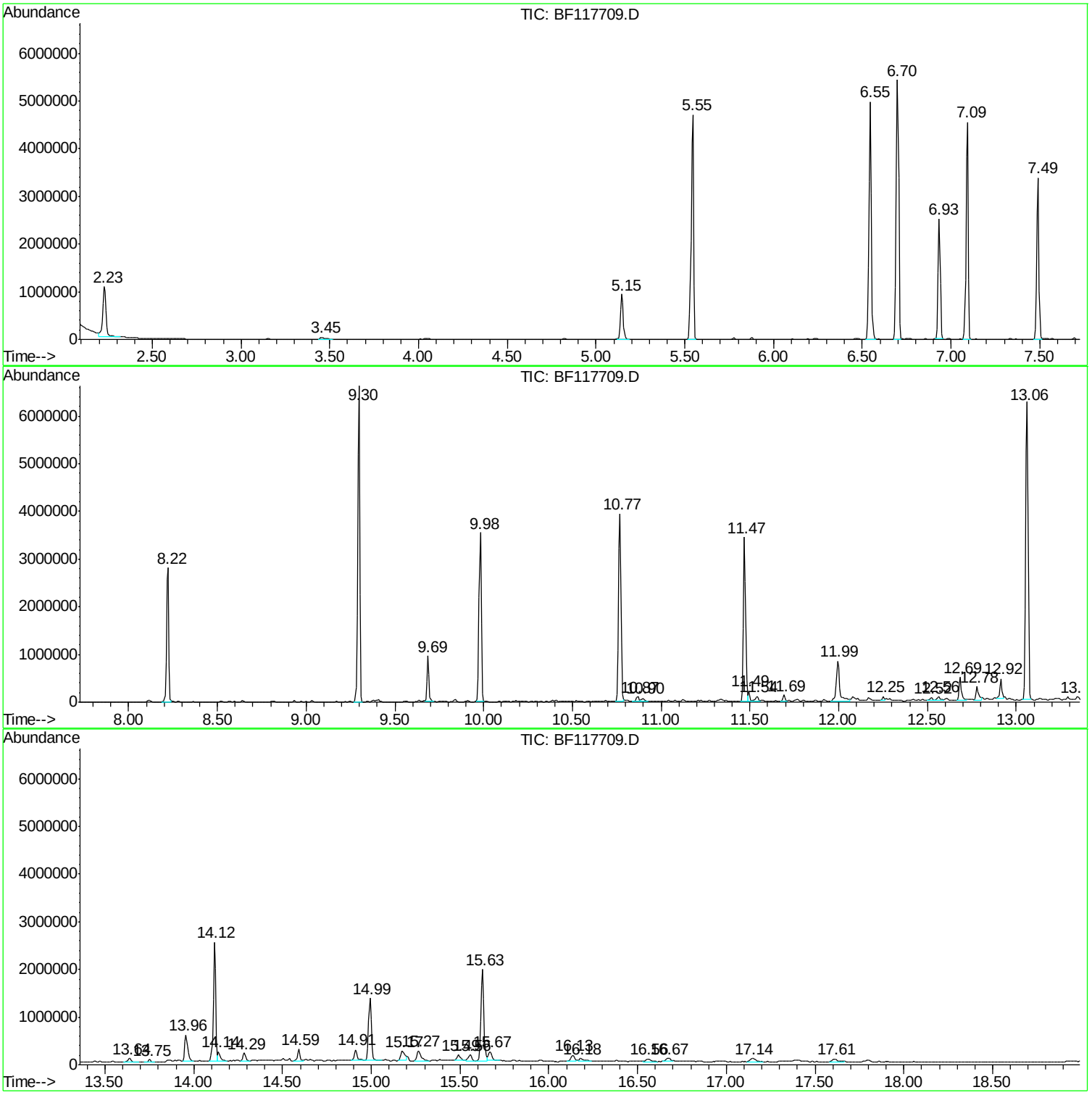
Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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 : BF117709.D
Acq On : 7 Nov 2019 17:19
Operator : JU
Sample : K5723-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

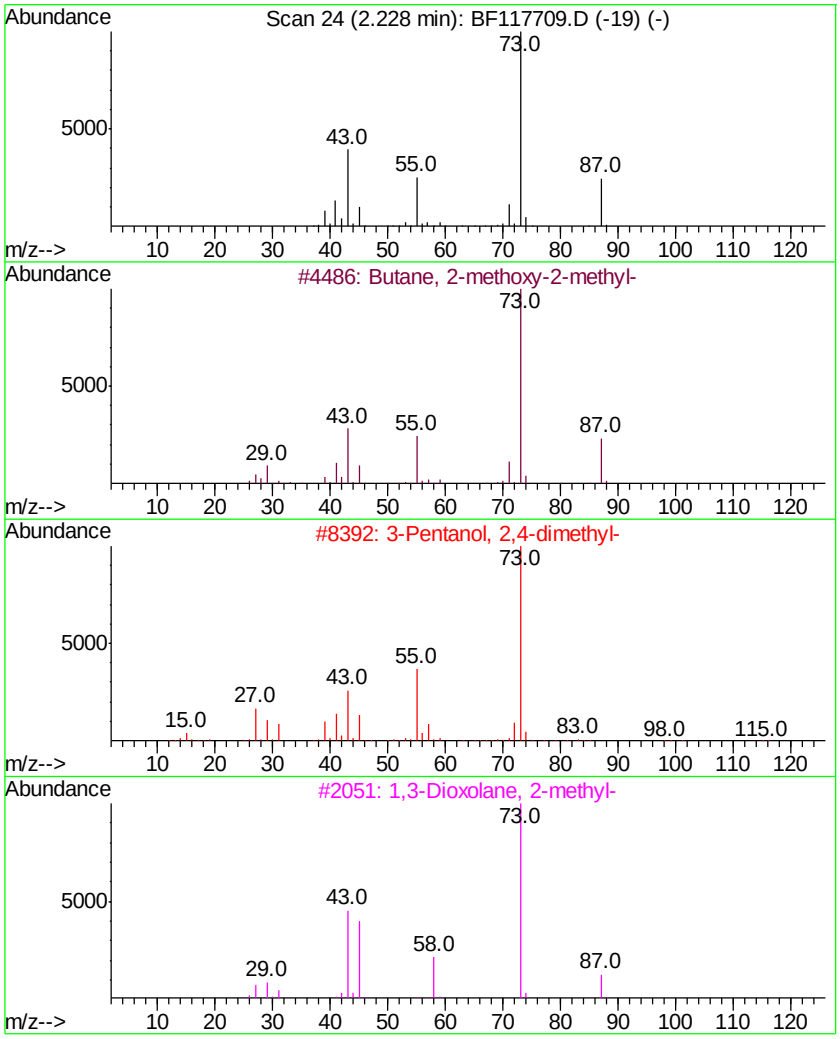
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

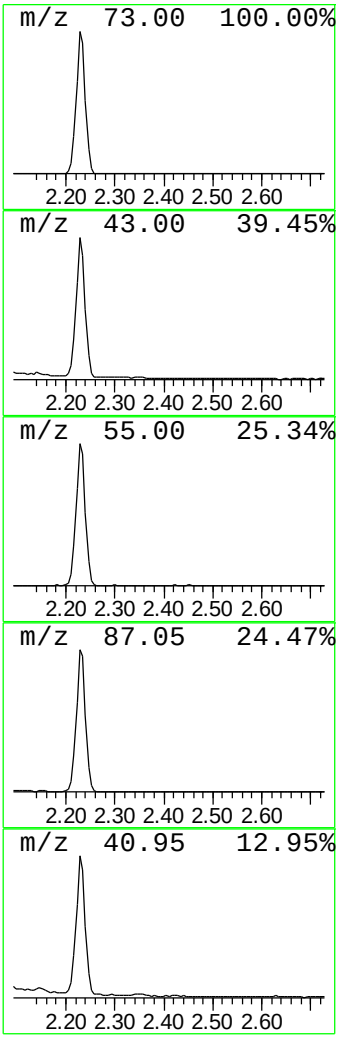
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	15.66 ng	1487690	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

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Operator : JU
Sample : K5723-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

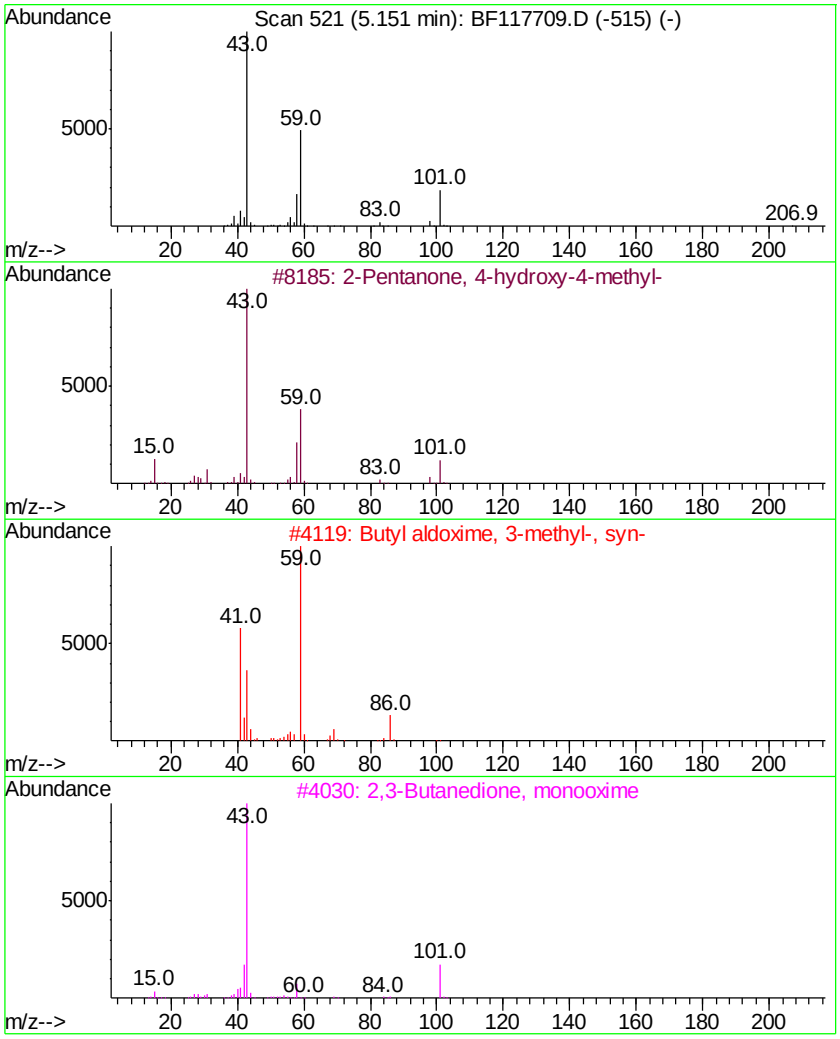
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

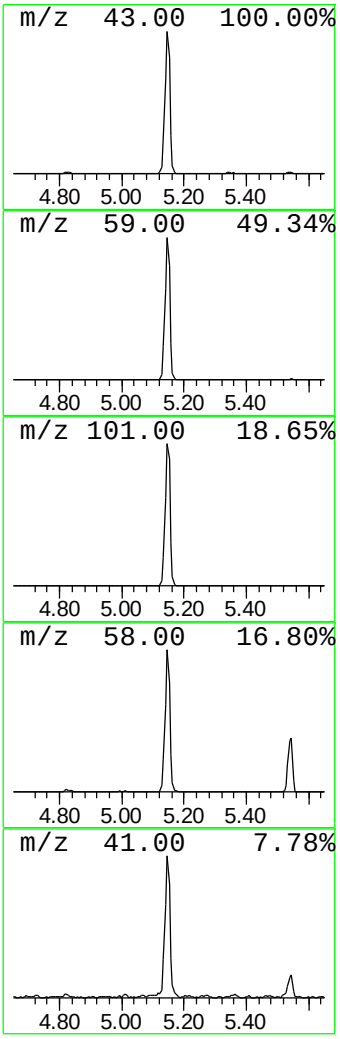
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	10.93 ng	1038600	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

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Acq On : 7 Nov 2019 17:19
Operator : JU
Sample : K5723-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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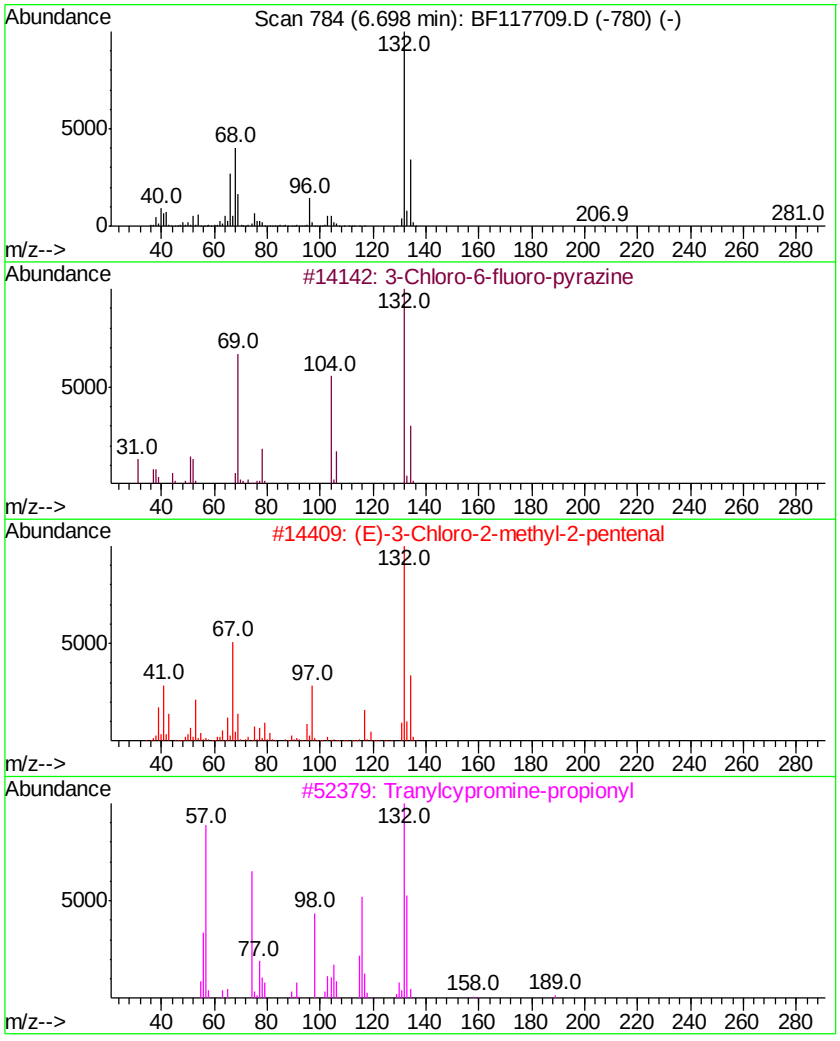
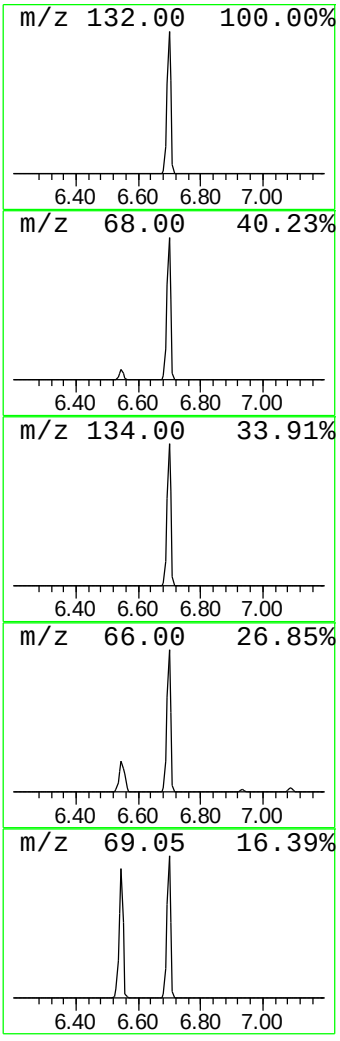
****

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	51.52 ng	4894450	1,4-Dichlorobenzene-d4	6.93

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	12
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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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

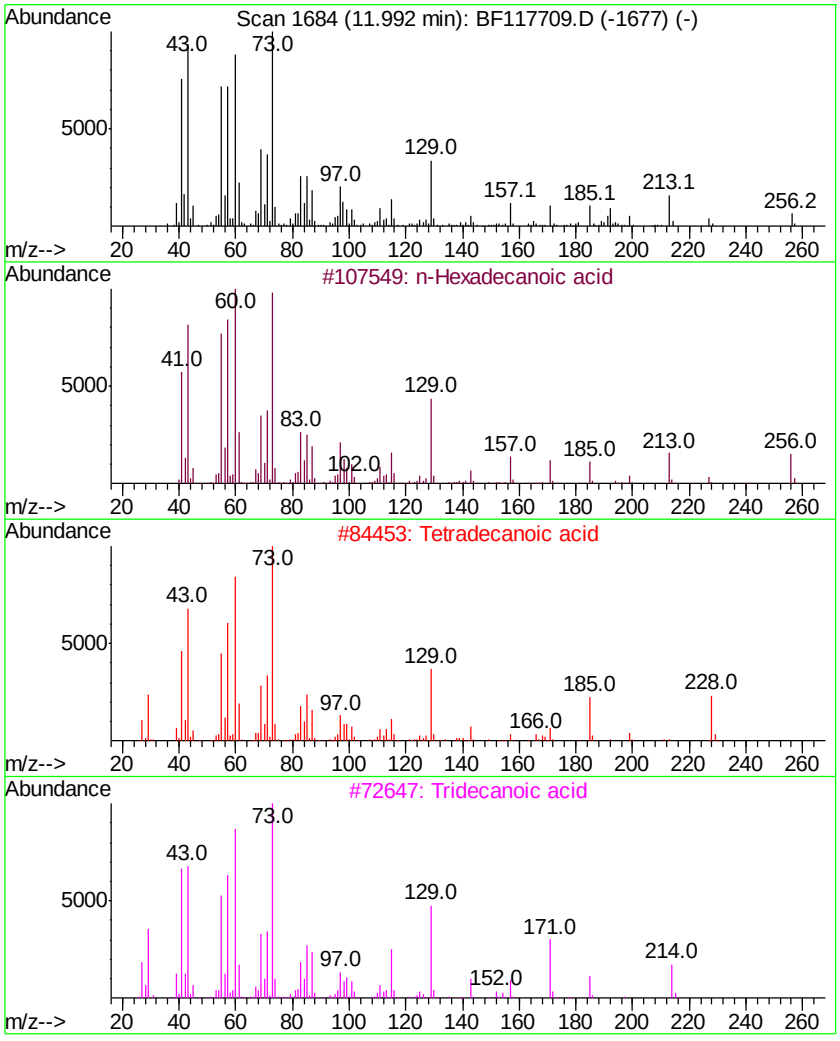
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

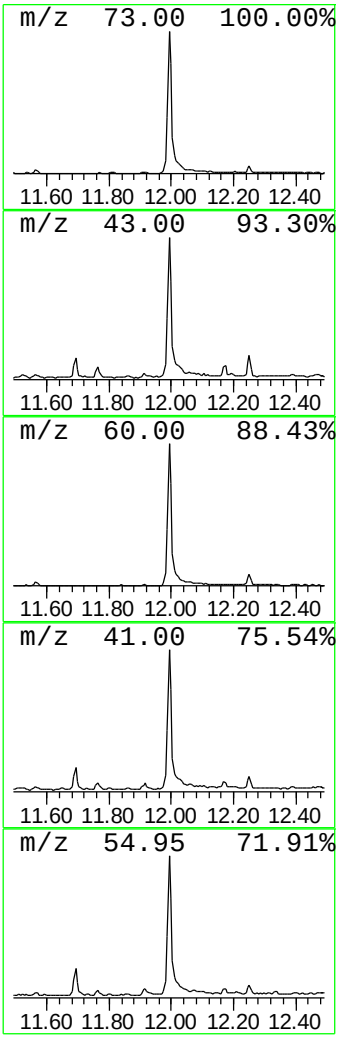
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	7.16 ng	1042060	Phenanthrene-d10	11.47

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	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	95
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Instrument : BNA_F
ClientSampleId : 7-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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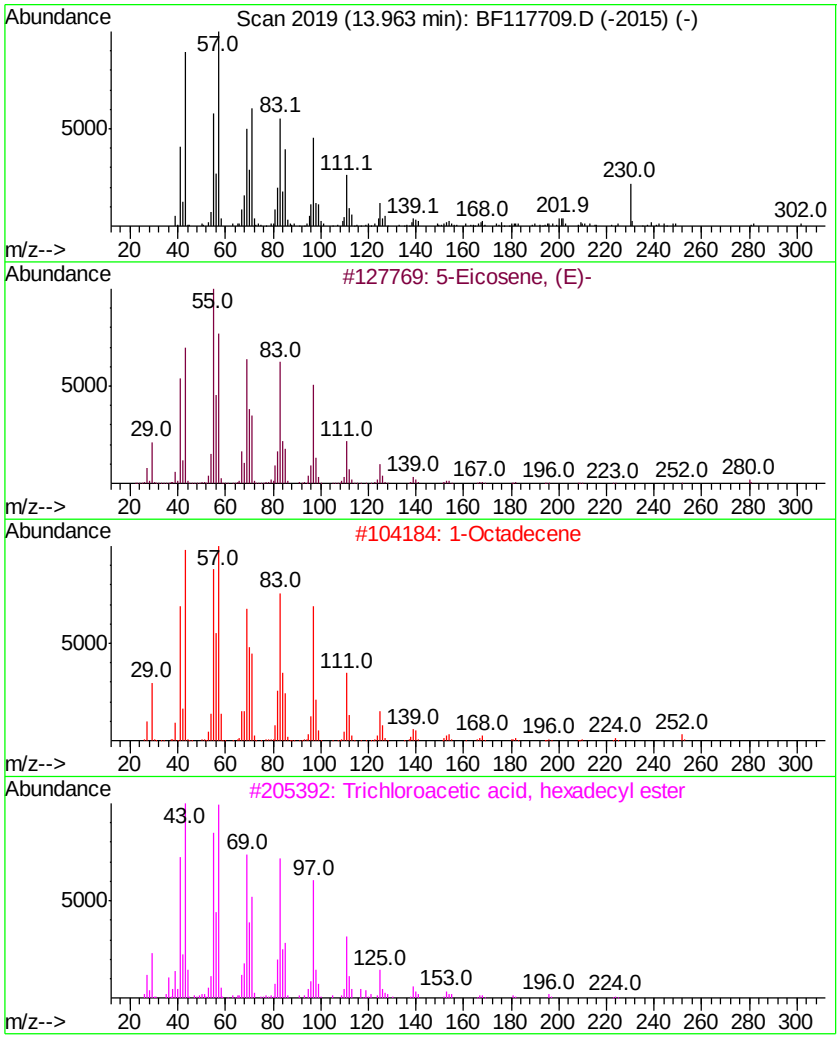
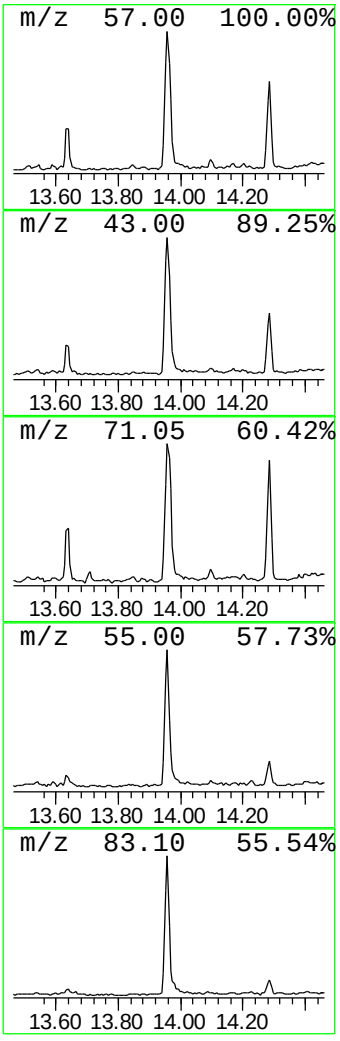
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.00 ng	604722	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Octadecene	252	C18H36	000112-88-9	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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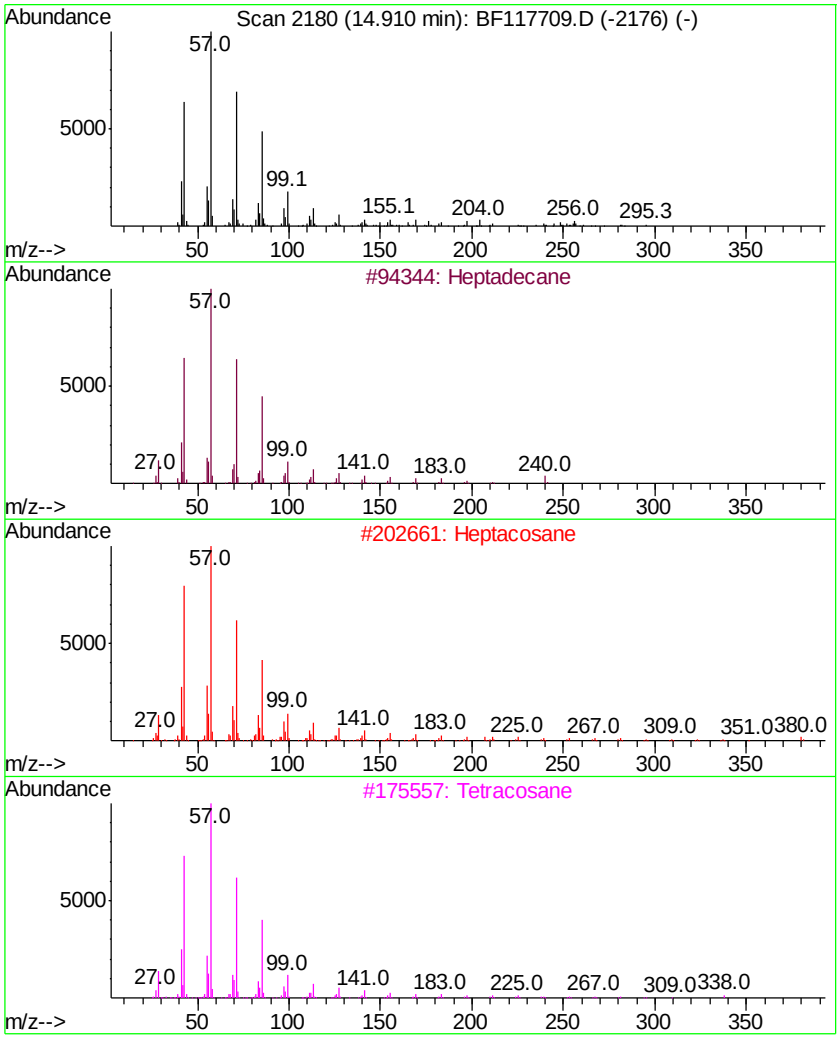
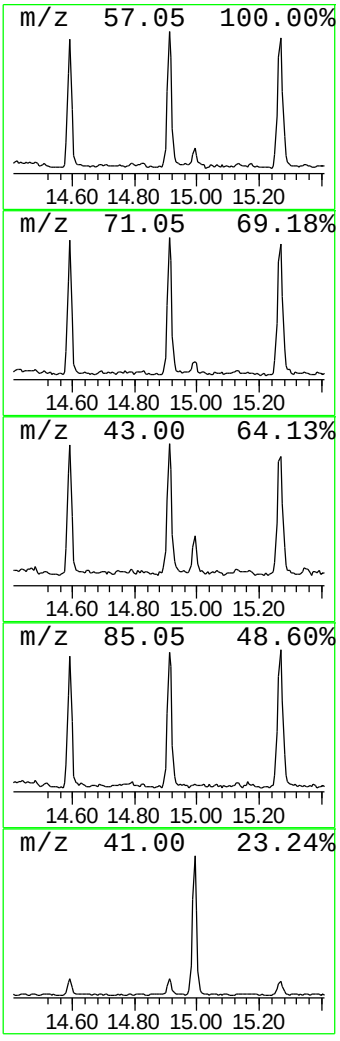
Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	2.25 ng	262955	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octadecane	254	C18H38	000593-45-3	87





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Instrument : BNA_F
ClientSampleId : 7-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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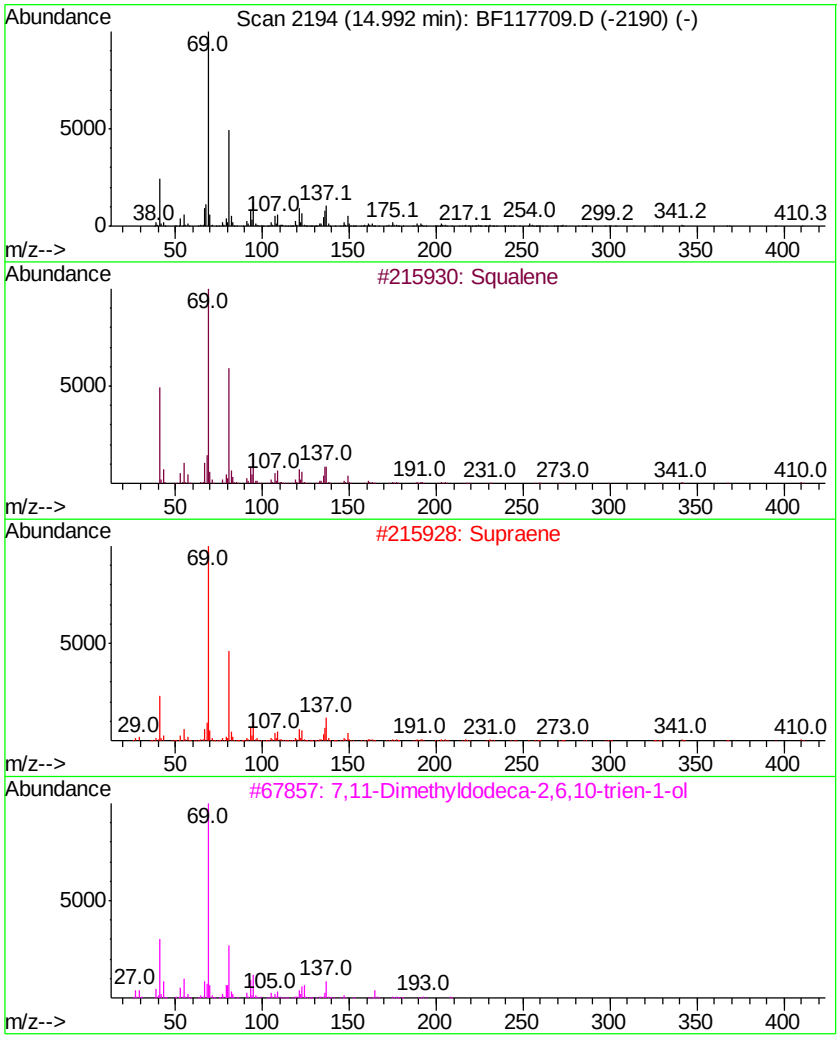
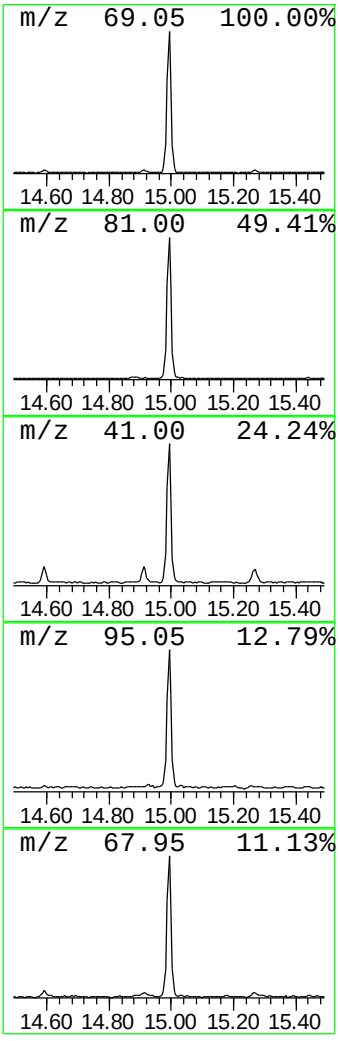
Peak Number 8 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	11.40 ng	1329380	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53





Library Search Compound Report

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Data File : BF117709.D
Acq On : 7 Nov 2019 17:19
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Sample : K5723-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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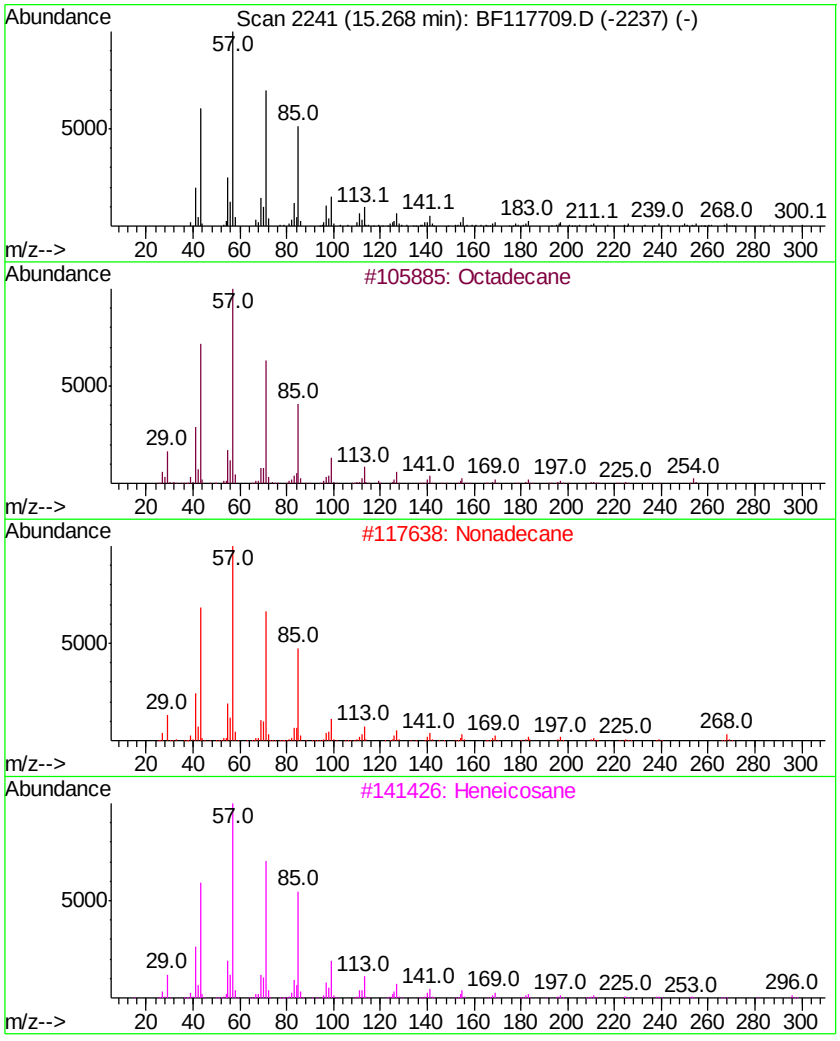
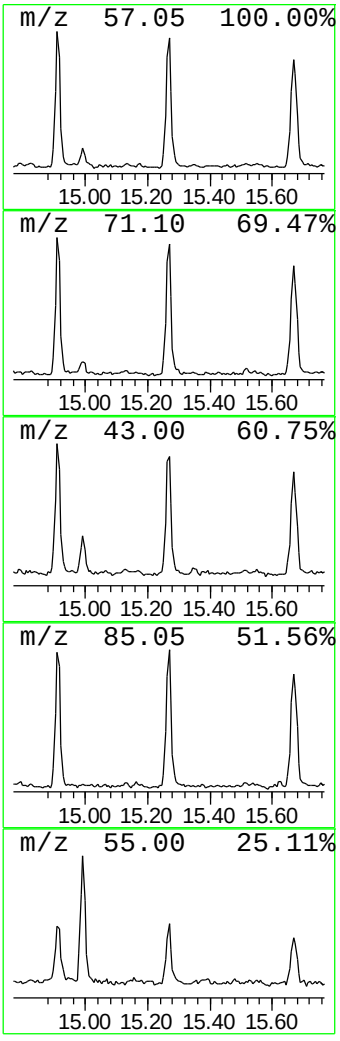
Peak Number 9 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.70 ng	314884	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Nonadecane	268	C19H40	000629-92-5	95
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110719\
Data File : BF117709.D
Acq On : 7 Nov 2019 17:19
Operator : JU
Sample : K5723-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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...	2.23	15.7	ng	1487690	1	6.93	1900040	20.0
2-Pentanone, 4-hy...	5.15	10.9	ng	1038600	1	6.93	1900040	20.0
unknown6.70	6.70	51.5	ng	4894450	1	6.93	1900040	20.0
n-Hexadecanoic acid	11.99	7.2	ng	1042060	4	11.47	2912130	20.0
5-Eicosene, (E)-	13.96	5.0	ng	604722	5	14.12	2417640	20.0
Heptadecane	14.91	2.3	ng	262955	6	15.63	2333200	20.0
Squalene	14.99	11.4	ng	1329380	6	15.63	2333200	20.0
Octadecane	15.27	2.7	ng	314884	6	15.63	2333200	20.0