LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109238.D
Acq On : 22 Sep 2018 22:49
Operator : JU/SJ
Sample : J4777-29 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-04-092018-C

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-BF092218.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	4.887	473	476	484	rVB	48119	53516	3.73%	0.323%
2	5.310	543	548	551	rBV	1221557	1146557	80.00%	6.929%
3	6.340	718	723	726	rBV	1458674	1253780	87.49%	7.577%
4	6.475	741	746	749	rBV	1345757	1259608	87.89%	7.612%
5	6.704	782	785	789	rBV	873066	695822	48.55%	4.205%
6	6.863	808	812	815	rBV	1267738	999818	69.76%	6.042%
7	6.987	830	833	838	rVB	35083	37434	2.61%	0.226%
8	7.263	871	880	883	rBV	975489	800618	55.86%	4.838%
9	7.363	892	897	901	rBV5	28879	44661	3.12%	0.270%
10	7.504	919	921	928	rVB3	37122	55016	3.84%	0.332%
11	7.634	936	943	948	rVB7	40433	81687	5.70%	0.494%
12	7.681	948	951	955	rBV3	15479	26861	1.87%	0.162%
13	7.763	962	965	970	rVB5	25787	28928	2.02%	0.175%
14	7.822	973	975	979	rVB3	31073	33765	2.36%	0.204%
15	7.869	979	983	984	rBV3	19023	20571	1.44%	0.124%
16	7.987	999	1003	1006	rBV	1151048	933131	65.11%	5.639%
17	8.069	1015	1017	1019	rBV	47505	36536	2.55%	0.221%
18	8.087	1019	1020	1023	rVB3	24418	19379	1.35%	0.117%
19	8.122	1023	1026	1028	rVB3	30049	28880	2.02%	0.175%
20	8.151	1028	1031	1032	rBV2	20838	21950	1.53%	0.133%
21	8.169	1032	1034	1038	rVV5	29654	31974	2.23%	0.193%
22	8.204	1038	1040	1043	rVB	148865	108905	7.60%	0.658%
23	8.287	1051	1054	1057	rVB4	57078	68261	4.76%	0.413%
24	8.322	1057	1060	1062	rBV4	26493	26441	1.84%	0.160%
25	8.345	1062	1064	1066	rBV3	33233	32350	2.26%	0.195%
26	8.428	1075	1078	1082	rBV3	78716	125113	8.73%	0.756%
27	8.498	1088	1090	1093	rVB2	55432	42262	2.95%	0.255%
28	8.539	1093	1097	1100	rBV2	103516	102636	7.16%	0.620%
29	8.598	1104	1107	1112	rBV5	37165	59497	4.15%	0.360%
30	8.686	1120	1122	1126	rVB4	67373	81420	5.68%	0.492%
31	8.739	1128	1131	1133	rBV3	27071	33973	2.37%	0.205%
32	8.875	1152	1154	1158	rBV3	30696	43954	3.07%	0.266%
33	8.986	1170	1173	1175	rVB3	33769	28268	1.97%	0.171%
34	9.022	1176	1179	1182	rVB	206277	179775	12.54%	1.086%

LSC Area Percent Report

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Acq On : 22 Sep 2018 22:49
Operator : JU/SJ
Sample : J4777-29 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-04-092018-C

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.063	1182	1186	1189	rBV	1918066	1433133	100.00%	8.661%
36	9.157	1198	1202	1206	rBV3	139518	160256	11.18%	0.968%
37	9.204	1206	1210	1213	rBV2	60889	77992	5.44%	0.471%
38	9.269	1219	1221	1224	rBV3	29559	22484	1.57%	0.136%
39	9.328	1226	1231	1233	rBV5	36061	56263	3.93%	0.340%
40	9.422	1245	1247	1250	rBV3	23030	27100	1.89%	0.164%
41	9.457	1250	1253	1255	rVV	351231	281707	19.66%	1.702%
42	9.481	1255	1257	1259	rVB2	71461	51809	3.62%	0.313%
43	9.622	1279	1281	1285	rVB4	49663	44373	3.10%	0.268%
44	9.657	1285	1287	1290	rBV3	50628	44370	3.10%	0.268%
45	9.686	1290	1292	1294	rVV3	28070	25252	1.76%	0.153%
46	9.739	1296	1301	1304	rVV	1066490	988538	68.98%	5.974%
47	9.786	1307	1309	1314	rVV5	34017	52183	3.64%	0.315%
48	9.845	1316	1319	1324	rVB4	59797	82731	5.77%	0.500%
49	9.910	1327	1330	1331	rVV2	31347	32938	2.30%	0.199%
50	9.928	1331	1333	1339	rVB5	59853	83618	5.83%	0.505%
51	9.975	1339	1341	1344	rVB3	35635	33292	2.32%	0.201%
52	10.010	1344	1347	1350	rBV2	84866	72593	5.07%	0.439%
53	10.057	1353	1355	1357	rVV2	34831	26279	1.83%	0.159%
54	10.204	1378	1380	1382	rVV2	27095	20184	1.41%	0.122%
55	10.233	1382	1385	1390	rVB4	60943	71059	4.96%	0.429%
56	10.304	1395	1397	1401	rVV2	50034	50453	3.52%	0.305%
57	10.345	1402	1404	1406	rVB3	38726	30596	2.13%	0.185%
58	10.375	1406	1409	1411	rBV2	29484	33156	2.31%	0.200%
59	10.404	1411	1414	1418	rVB3	53647	58130	4.06%	0.351%
60	10.486	1425	1428	1430	rBV3	34663	36247	2.53%	0.219%
61	10.516	1430	1433	1438	rVB	708117	659398	46.01%	3.985%
62	10.651	1453	1456	1457	rBV3	35853	33169	2.31%	0.200%
63	10.722	1466	1468	1470	rBV3	34795	29597	2.07%	0.179%
64	10.804	1479	1482	1484	rBV3	20049	21221	1.48%	0.128%
65	11.128	1535	1537	1541	rVB	46741	43834	3.06%	0.265%
66	11.210	1548	1551	1554	rBV	889696	761233	53.12%	4.600%
67	11.569	1610	1612	1618	rVB6	21983	30991	2.16%	0.187%
68	11.622	1618	1621	1627	rBV4	14201	24124	1.68%	0.146%
69	11.751	1640	1643	1647	rVB5	19731	22491	1.57%	0.136%
70	11.822	1652	1655	1658	rBV4	16153	22214	1.55%	0.134%
71	12.139	1706	1709	1714	rBV2	22741	28232	1.97%	0.171%

LSC Area Percent Report

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Sample : J4777-29 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-04-092018-C

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.416	1754	1756	1759	rBV	41093	32127	2.24%	0.194%
73	12.469	1762	1765	1769	rVB6	20181	25135	1.75%	0.152%
74	12.645	1792	1795	1797	rBV	24027	23777	1.66%	0.144%
75	12.792	1817	1820	1823	rBV	1216425	958197	66.86%	5.790%
76	12.974	1849	1851	1856	rBV5	25172	28603	2.00%	0.173%
77	13.039	1860	1862	1865	rVB2	32339	26768	1.87%	0.162%
78	13.380	1918	1920	1924	rBV4	31899	34633	2.42%	0.209%
79	13.710	1973	1976	1981	rBV4	50406	70665	4.93%	0.427%
80	13.839	1994	1998	2001	rBV	676818	631799	44.09%	3.818%
81	14.021	2027	2029	2033	rBV	44982	43249	3.02%	0.261%
82	14.621	2129	2131	2136	rBV3	67606	92462	6.45%	0.559%
83	15.239	2232	2236	2240	rVB	432632	463852	32.37%	2.803%

Sum of corrected areas: 16547854

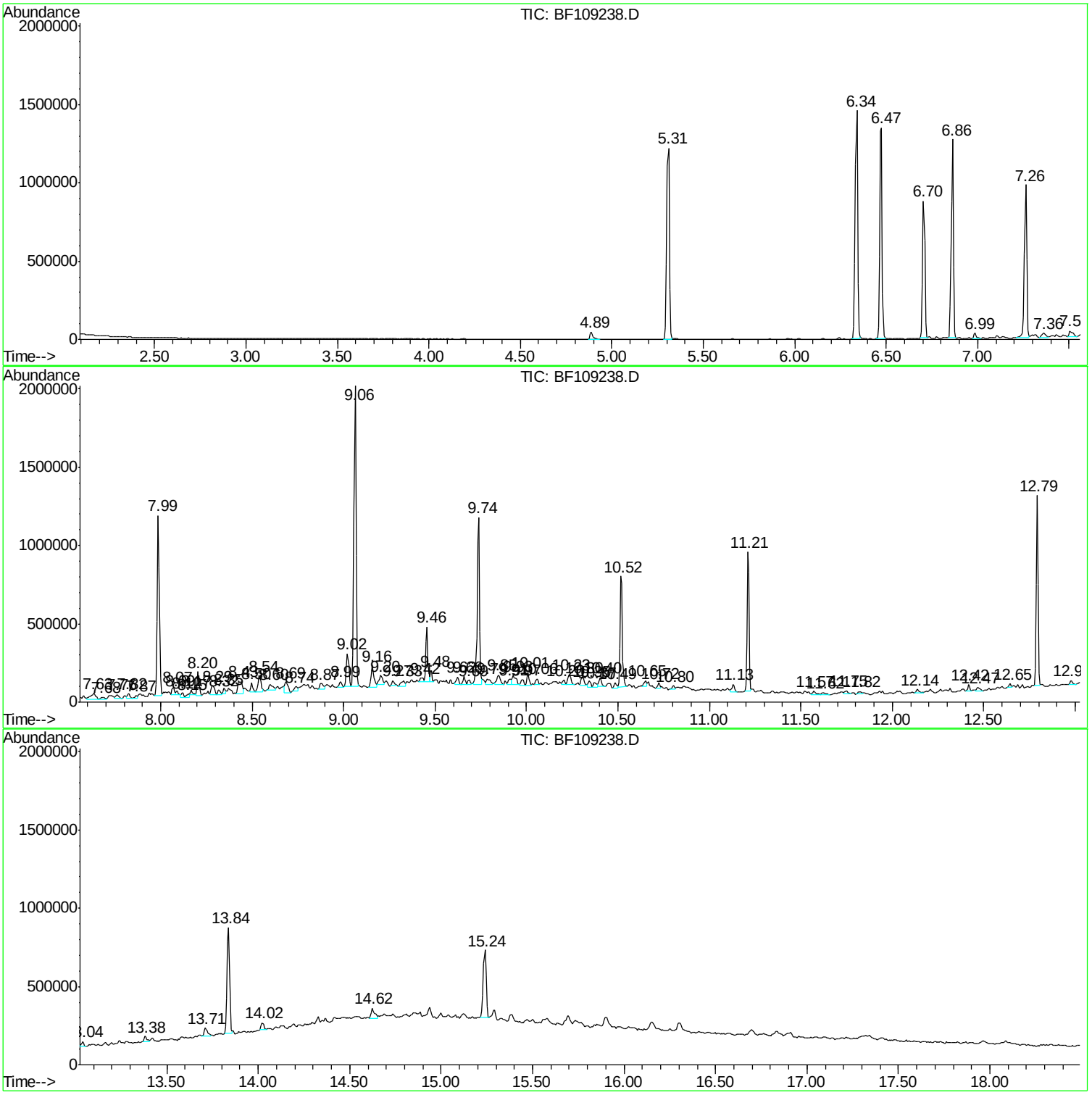
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109238.D
Acq On : 22 Sep 2018 22:49
Operator : JU/SJ
Sample : J4777-29 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-04-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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\BF092218\
Data File : BF109238.D
Acq On : 22 Sep 2018 22:49
Operator : JU/SJ
Sample : J4777-29 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-04-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

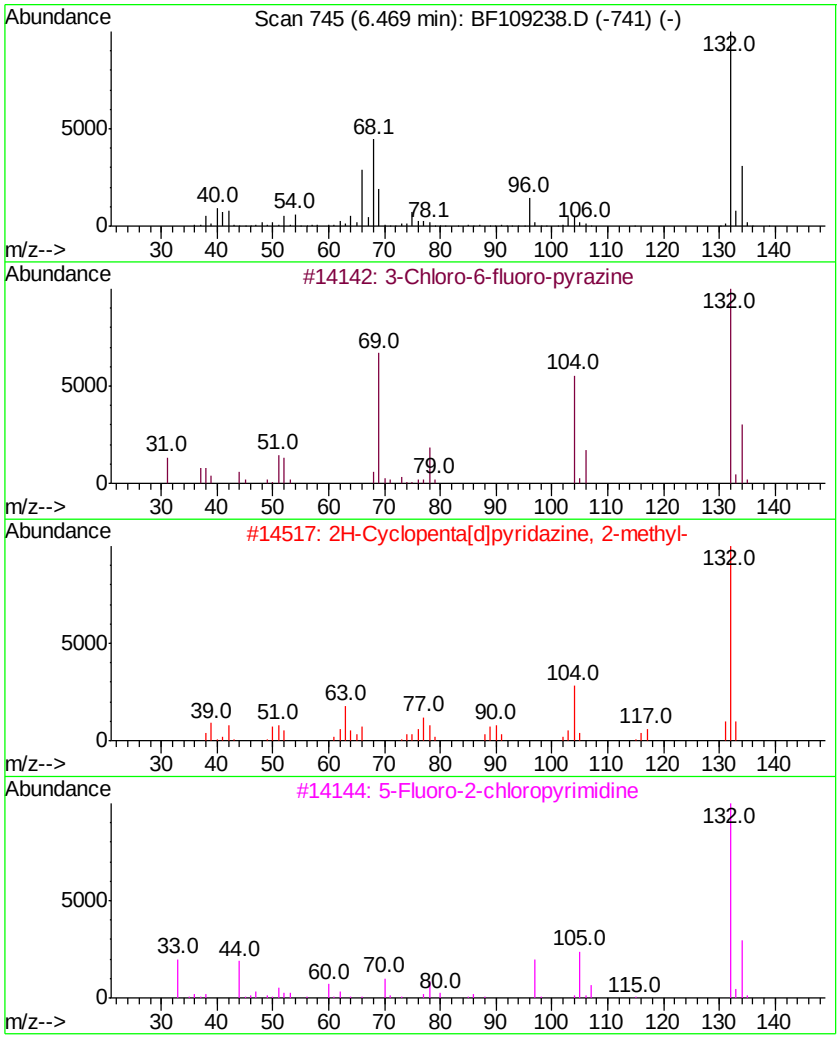
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

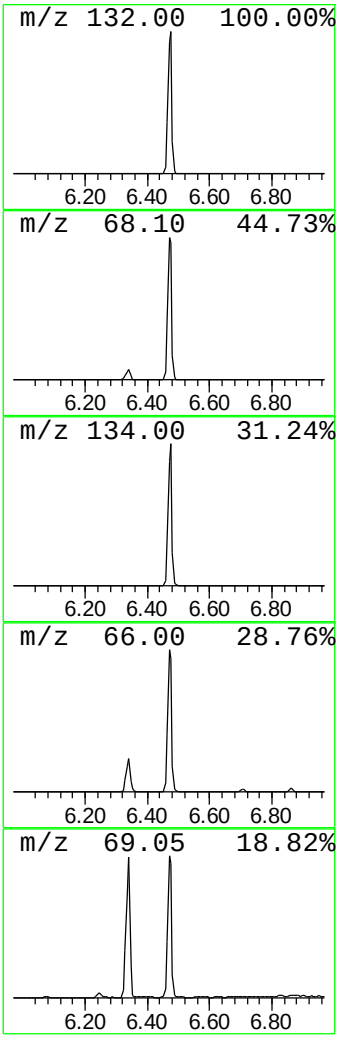
****

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	36.20 ng	1259610	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





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Instrument : BNA_F
ClientSampleId : PL-04-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

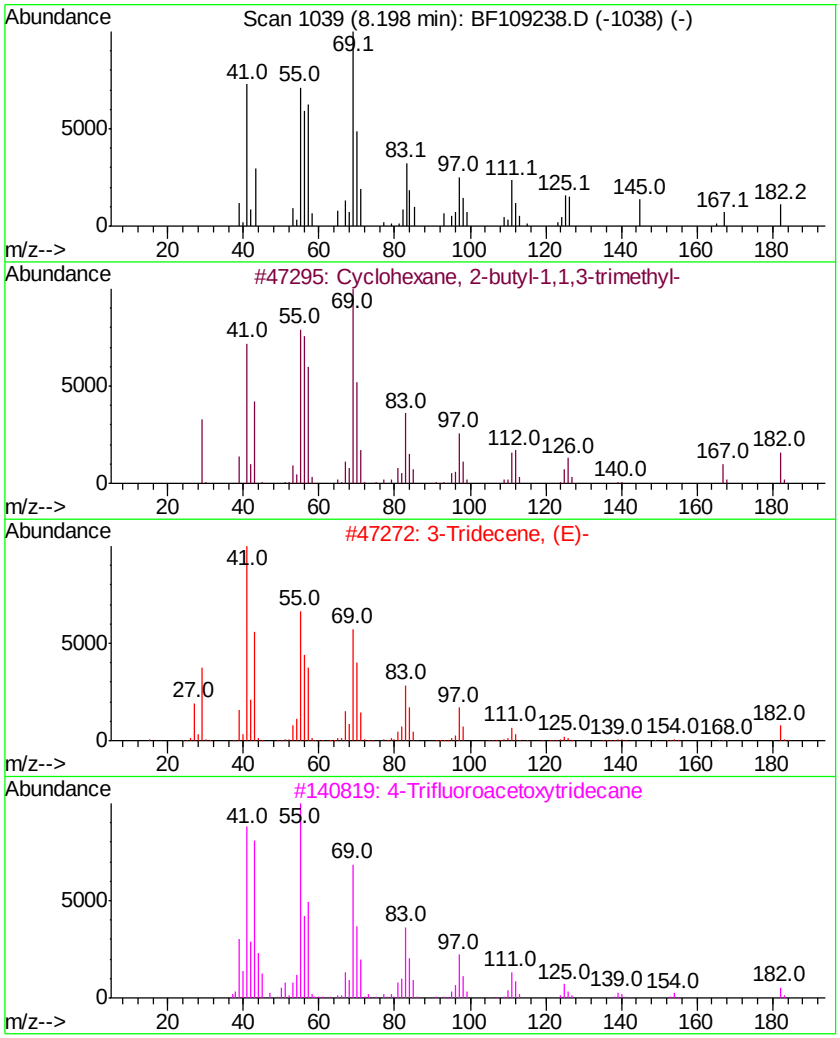
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

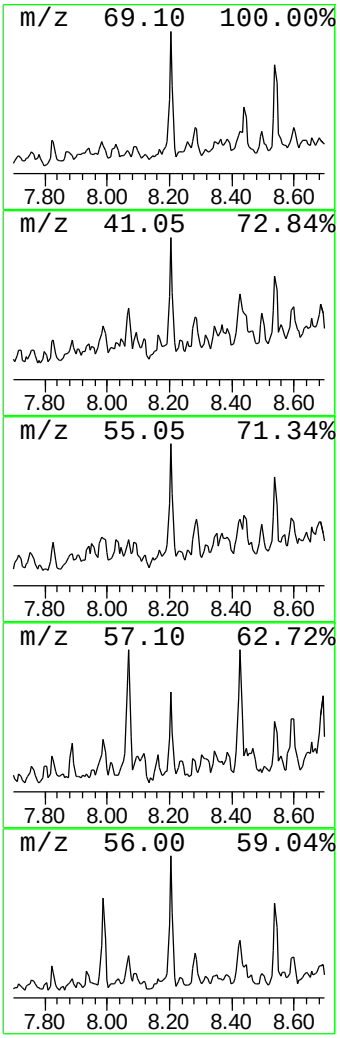
****

Peak Number 3 Cyclohexane, 2-butyl-1,1,3-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.20	2.33 ng	108905	Naphthalene-d8	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	96
2	3-Tridecene, (E)-	182	C13H26	041446-57-5	87
3	4-Trifluoroacetoxytridecane	296	C15H27F3O2	1000245-47-3	86
4	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	58
5	3-Tridecene, (Z)-	182	C13H26	041446-53-1	55





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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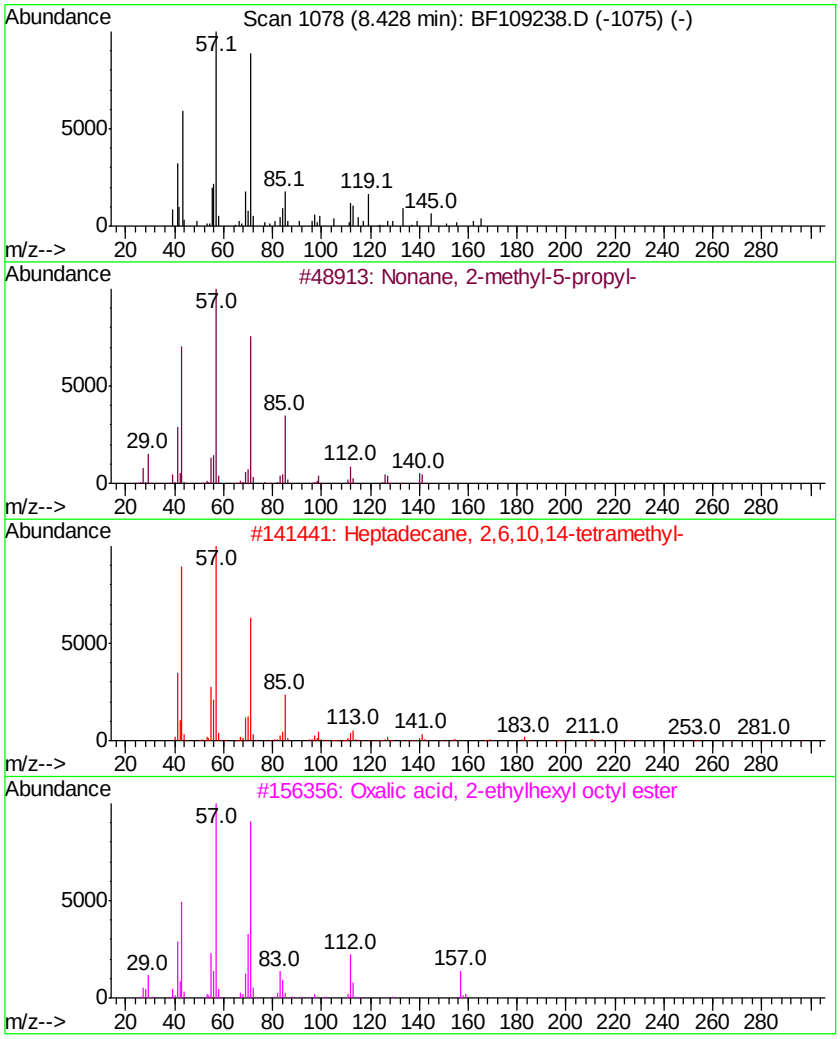
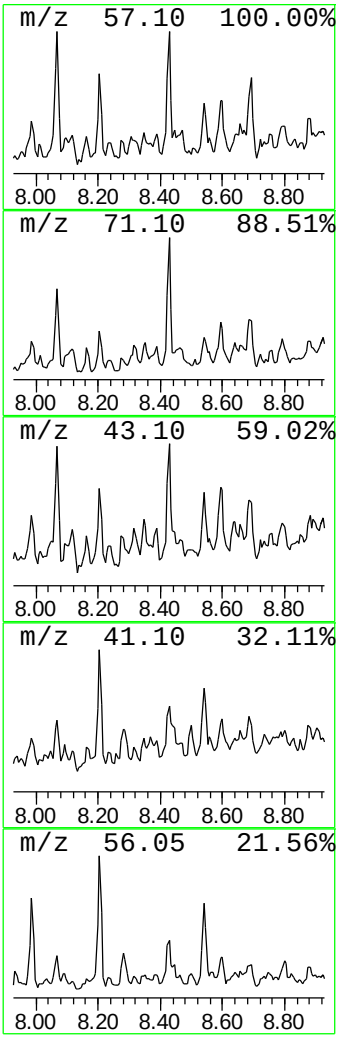
****

Peak Number 4 Nonane, 2-methyl-5-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.43	2.68 ng	125113	Naphthalene-d8	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	59
2	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	59
3	Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	53
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	53
5	Oxalic acid, ethyl neopentyl ester	188	C9H16O4	1000309-72-4	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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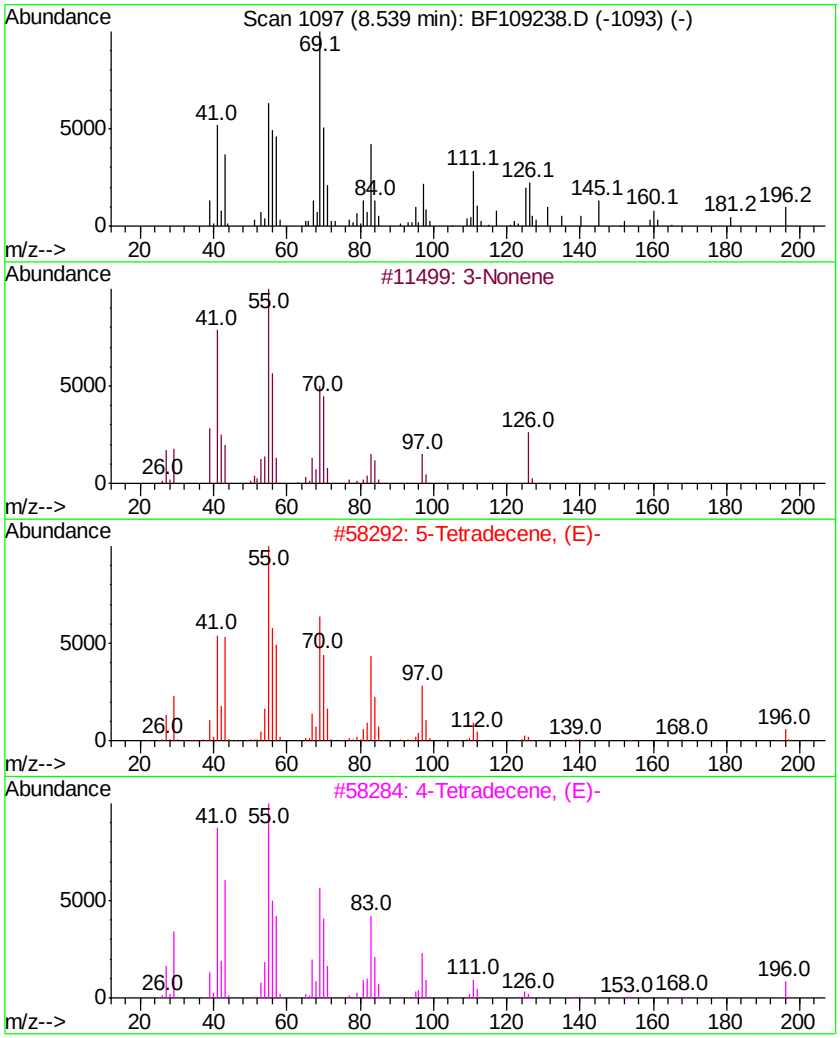
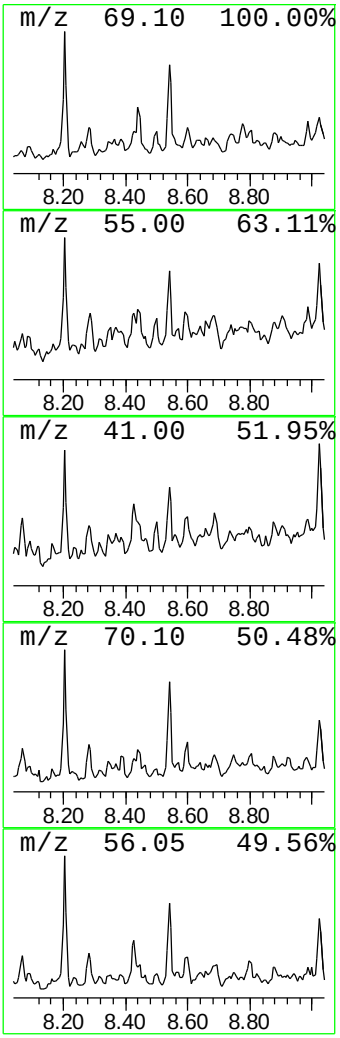
****

Peak Number 5 unknown8.54 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.54	2.20 ng	102636	Naphthalene-d8	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Nonene	126	C9H18	020063-77-8	46
2	5-Tetradecene, (E)-	196	C14H28	041446-66-6	46
3	4-Tetradecene, (E)-	196	C14H28	041446-78-0	43
4	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	43
5	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	43





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Instrument : BNA_F
ClientSampleId : PL-04-092018-C

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

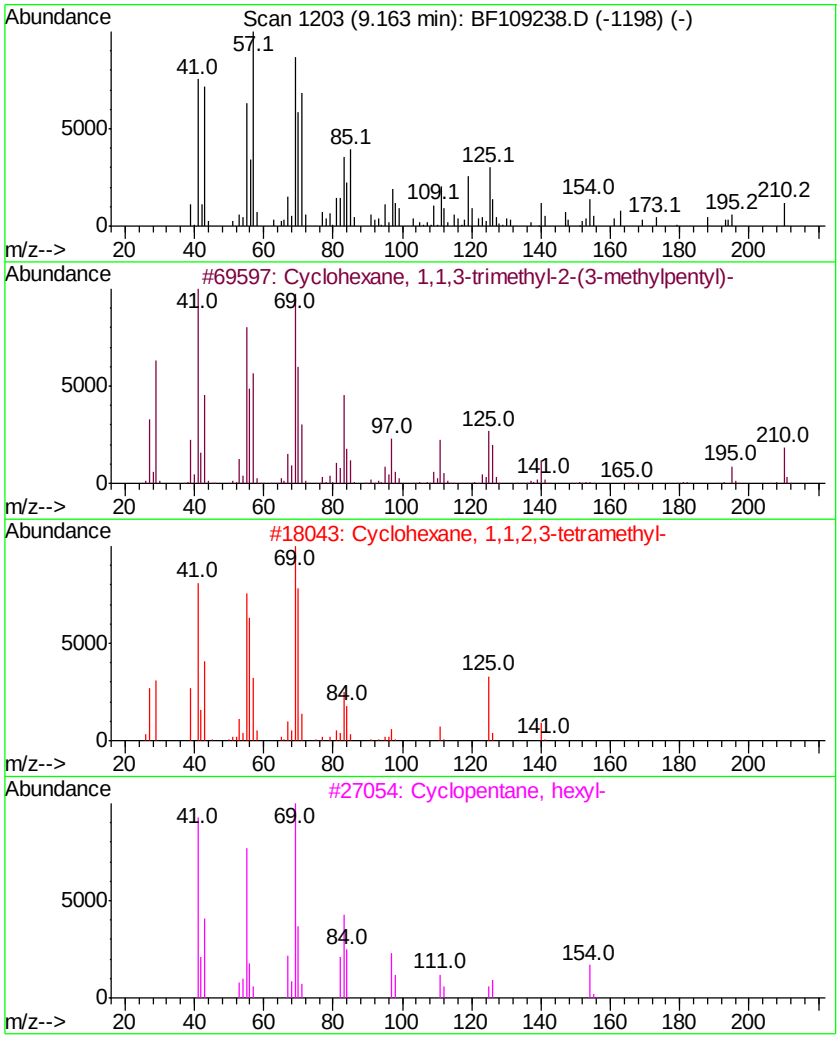
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

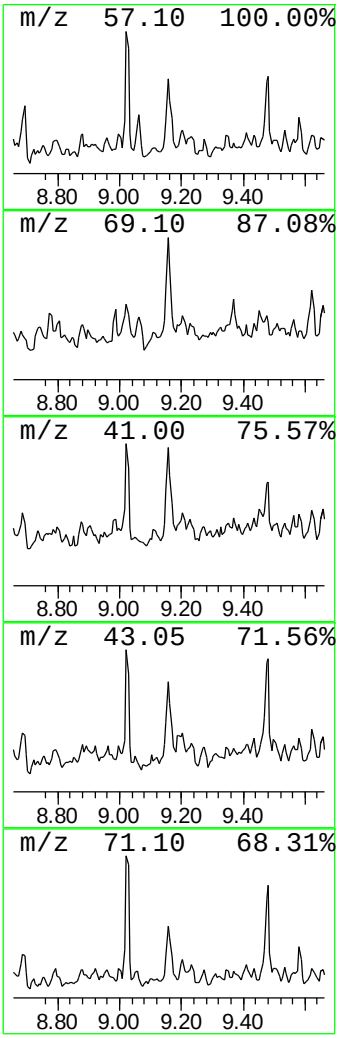
****

Peak Number 6 Cyclohexane, 1,1,3-trimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	3.24 ng	160256	Acenaphthene-d10	9.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-2-(...	210	C15H30	054965-05-8	83
2	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	58
3	Cyclopentane, hexyl-	154	C11H22	004457-00-5	50
4	5-Undecene, (E)-	154	C11H22	000764-97-6	49
5	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	49





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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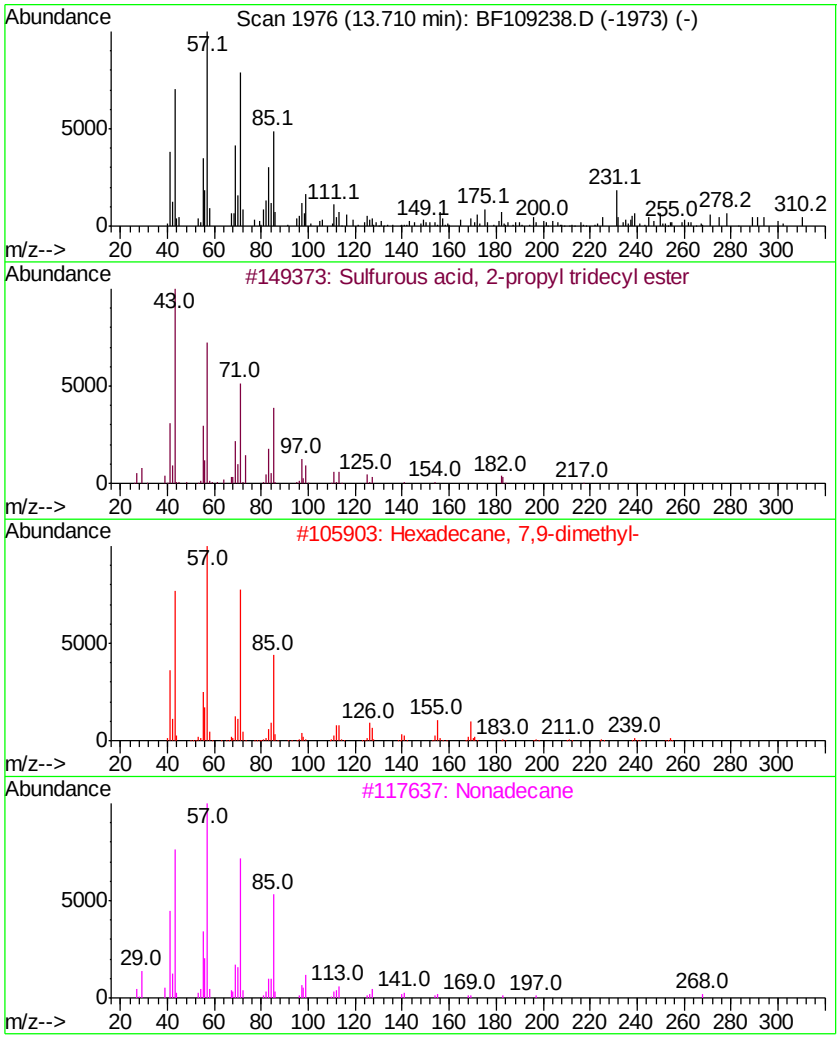
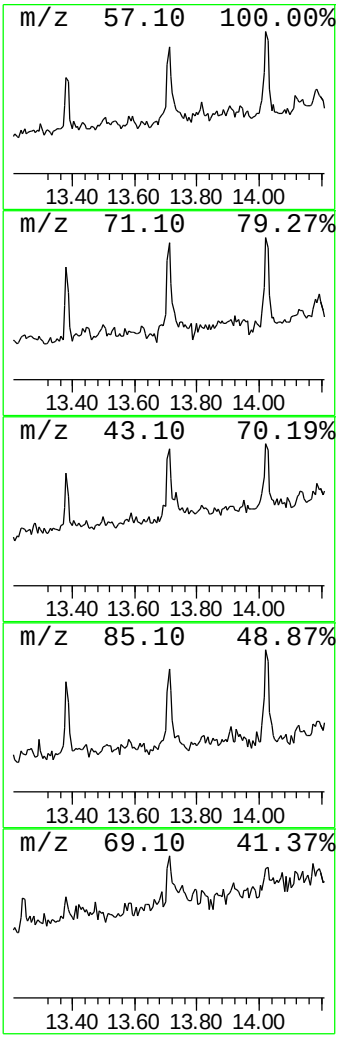
****

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	2.24 ng	70665	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	68
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	68
3	Nonadecane	268	C19H40	000629-92-5	68
4	10-Methylnonadecane	282	C20H42	056862-62-5	68
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	68





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Data File : BF109238.D
Acq On : 22 Sep 2018 22:49
Operator : JU/SJ
Sample : J4777-29 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-04-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

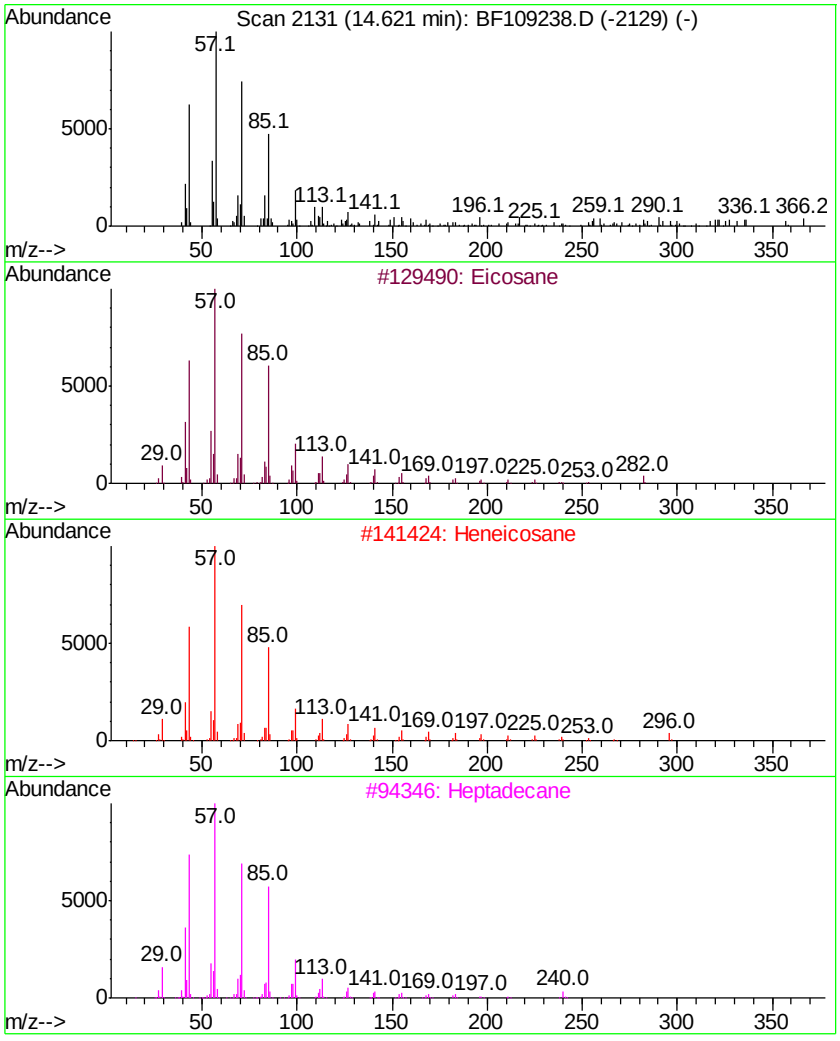
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

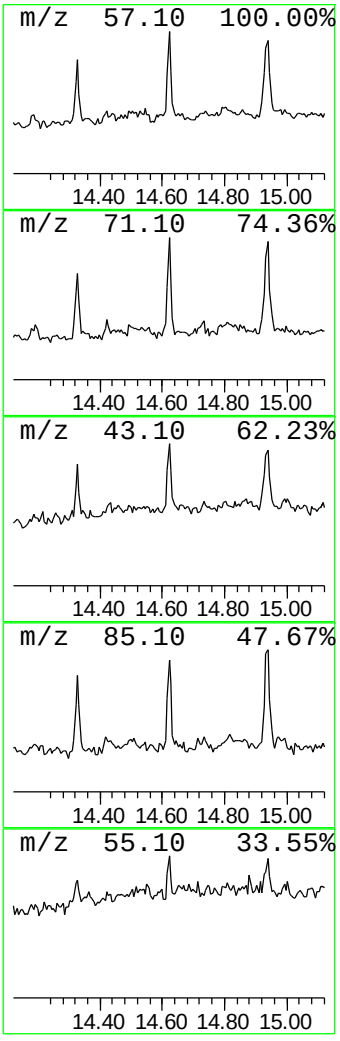
****

Peak Number 8 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.99 ng	92462	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Heneicosane	296	C21H44	000629-94-7	89
3	Heptadecane	240	C17H36	000629-78-7	89
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	89
5	Nonadecane	268	C19H40	000629-92-5	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092218\
Data File : BF109238.D
Acq On : 22 Sep 2018 22:49
Operator : JU/SJ
Sample : J4777-29 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-04-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
unknown6.47	6.47	36.2	ng	1259610	1	6.70	695822	20.0
Cyclohexane, 2-bu...	8.20	2.3	ng	108905	2	7.99	933131	20.0
Nonane, 2-methyl-...	8.43	2.7	ng	125113	2	7.99	933131	20.0
unknown8.54	8.54	2.2	ng	102636	2	7.99	933131	20.0
Cyclohexane, 1,1,...	9.16	3.2	ng	160256	3	9.74	988538	20.0
Sulfurous acid, 2...	13.71	2.2	ng	70665	5	13.84	631799	20.0
Eicosane	14.62	4.0	ng	92462	6	15.24	463852	20.0