LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097342.D
Acq On : 4 Aug 2017 3:08
Operator : SJ/JU
Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	3.069	197	201	213	rBV2	5051	11426	1.62%	0.136%
2	4.563	451	455	466	rBV	28475	47320	6.70%	0.562%
3	4.969	520	524	526	rBV2	12032	13545	1.92%	0.161%
4	5.040	533	536	554	rBV	308317	473005	66.95%	5.621%
5	5.246	568	571	575	rVB	13313	14880	2.11%	0.177%
6	6.116	716	719	734	rVB	372144	488384	69.13%	5.804%
7	6.222	734	737	743	rVV	497672	498724	70.59%	5.926%
8	6.269	743	745	748	rVB	9542	8496	1.20%	0.101%
9	6.445	772	775	784	rBV	663115	593431	84.00%	7.052%
10	6.598	798	801	811	rBV	340949	338000	47.84%	4.017%
11	7.016	869	872	879	rBV	246910	255368	36.15%	3.035%
12	7.069	879	881	886	rVB3	9840	10950	1.55%	0.130%
13	7.728	990	993	1001	rBV	848435	706500	100.00%	8.396%
14	8.339	1093	1097	1100	rBV	16488	14114	2.00%	0.168%
15	8.439	1110	1114	1121	rVB2	9362	12973	1.84%	0.154%
16	8.539	1128	1131	1135	rVB2	9135	12473	1.77%	0.148%
17	8.769	1167	1170	1172	rBV	12386	11320	1.60%	0.135%
18	8.804	1172	1176	1179	rBV	528955	436326	61.76%	5.185%
19	8.904	1188	1193	1197	rVB2	25432	25932	3.67%	0.308%
20	9.069	1215	1221	1223	rBV4	6396	10860	1.54%	0.129%
21	9.204	1241	1244	1246	rBV	32748	32608	4.62%	0.387%
22	9.334	1262	1266	1268	rVB2	10547	9223	1.31%	0.110%
23	9.428	1278	1282	1285	rBV	45480	40782	5.77%	0.485%
24	9.469	1285	1289	1293	rVV	725385	604566	85.57%	7.184%
25	9.498	1293	1294	1297	rVB	17096	11679	1.65%	0.139%
26	9.592	1306	1310	1314	rVB6	5615	8910	1.26%	0.106%
27	9.657	1317	1321	1322	rVV3	7803	9095	1.29%	0.108%
28	9.681	1322	1325	1328	rVB3	14122	17629	2.50%	0.209%
29	9.745	1334	1336	1339	rVB	15353	13098	1.85%	0.156%
30	9.781	1339	1342	1347	rBV5	8946	14803	2.10%	0.176%
31	9.922	1364	1366	1370	rVB	39396	32588	4.61%	0.387%
32	10.016	1378	1382	1385	rBV2	21906	20244	2.87%	0.241%
33	10.081	1389	1393	1398	rBV6	5935	10532	1.49%	0.125%
34	10.145	1398	1404	1406	rBV	19605	24379	3.45%	0.290%

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Misc :
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Instrument : BNA_F
ClientSampleId : JC-02-080117-E

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.257	1420	1423	1428	rBV	190166	170528	24.14%	2.026%
36	10.392	1442	1446	1453	rVB	40598	52307	7.40%	0.622%
37	10.586	1477	1479	1482	rBV2	10851	10030	1.42%	0.119%
38	10.716	1498	1501	1505	rVB4	7953	10293	1.46%	0.122%
39	10.839	1518	1522	1524	rBV	40052	34885	4.94%	0.415%
40	10.869	1524	1527	1530	rVB2	15001	15208	2.15%	0.181%
41	10.939	1536	1539	1542	rBV	582905	525873	74.43%	6.249%
42	10.963	1542	1543	1547	rVV	160583	109380	15.48%	1.300%
43	11.016	1550	1552	1556	rVB	46006	37587	5.32%	0.447%
44	11.180	1577	1580	1583	rBV	13707	15559	2.20%	0.185%
45	11.263	1588	1594	1600	rVV3	41676	55253	7.82%	0.657%
46	11.357	1607	1610	1615	rVB4	14565	17522	2.48%	0.208%
47	11.439	1621	1624	1627	rBV2	30534	32478	4.60%	0.386%
48	11.469	1627	1629	1633	rVB	34803	33210	4.70%	0.395%
49	11.522	1633	1638	1640	rBV2	15976	21118	2.99%	0.251%
50	11.551	1640	1643	1646	rVV	50088	55762	7.89%	0.663%
51	11.575	1646	1647	1650	rVB	21041	13332	1.89%	0.158%
52	11.669	1660	1663	1669	rBV2	32423	39544	5.60%	0.470%
53	11.733	1672	1674	1677	rBV	12948	14590	2.07%	0.173%
54	11.816	1685	1688	1689	rBV3	8107	8312	1.18%	0.099%
55	11.863	1694	1696	1698	rBV2	12397	12893	1.82%	0.153%
56	11.916	1703	1705	1708	rVV4	15232	16113	2.28%	0.191%
57	11.939	1708	1709	1713	rVB4	12704	11008	1.56%	0.131%
58	11.992	1714	1718	1720	rBV	36301	35139	4.97%	0.418%
59	12.027	1720	1724	1726	rVV4	19185	33258	4.71%	0.395%
60	12.051	1726	1728	1731	rVV2	42190	44467	6.29%	0.528%
61	12.080	1731	1733	1736	rVB4	16743	15948	2.26%	0.190%
62	12.110	1736	1738	1741	rVB4	14100	11894	1.68%	0.141%
63	12.145	1741	1744	1749	rBV	215549	191211	27.06%	2.272%
64	12.198	1750	1753	1758	rBV7	17821	26413	3.74%	0.314%
65	12.292	1767	1769	1774	rBV6	11719	17893	2.53%	0.213%
66	12.369	1778	1782	1785	rVV	190373	194118	27.48%	2.307%
67	12.422	1789	1791	1797	rVB3	51395	61952	8.77%	0.736%
68	12.522	1805	1808	1815	rVB	398065	364798	51.63%	4.335%
69	12.592	1817	1820	1824	rBV5	16318	29060	4.11%	0.345%
70	12.774	1848	1851	1854	rVB2	57261	54162	7.67%	0.644%
71	12.804	1854	1856	1860	rBV2	38115	45630	6.46%	0.542%

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Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.898	1869	1872	1874	rBV2	30827	33106	4.69%	0.393%
73	13.116	1906	1909	1912	rBV	68113	74445	10.54%	0.885%
74	13.445	1962	1965	1970	rVB2	80426	93678	13.26%	1.113%
75	13.563	1981	1985	1988	rBV	524912	532104	75.32%	6.323%
76	13.757	2016	2018	2023	rVB2	56765	48993	6.93%	0.582%
77	14.357	2117	2120	2123	rBV2	84322	88923	12.59%	1.057%
78	14.910	2210	2214	2217	rBV	246853	271079	38.37%	3.221%

Sum of corrected areas: 8415219

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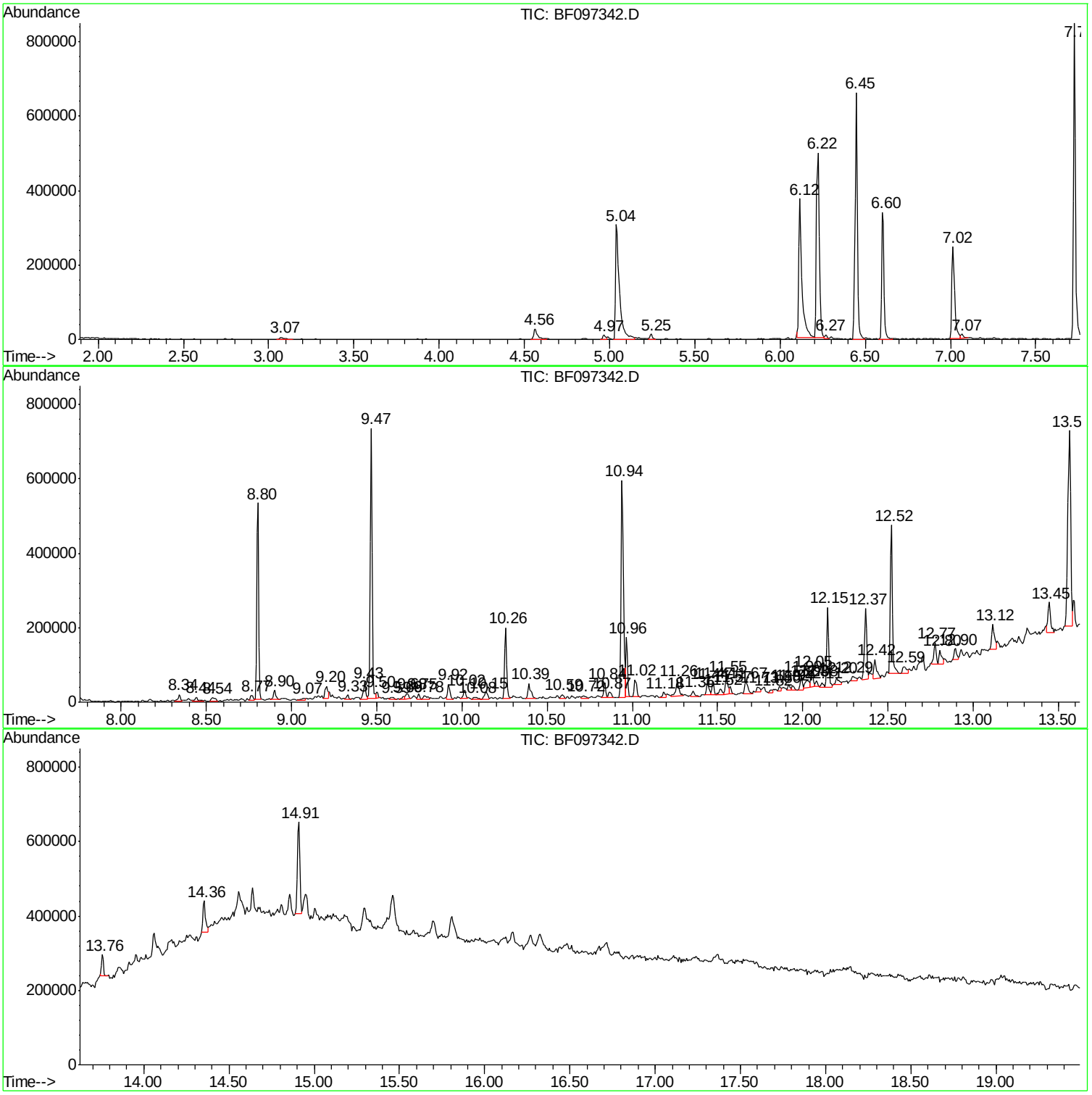
Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097342.D
Acq On : 4 Aug 2017 3:08
Operator : SJ/JU
Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

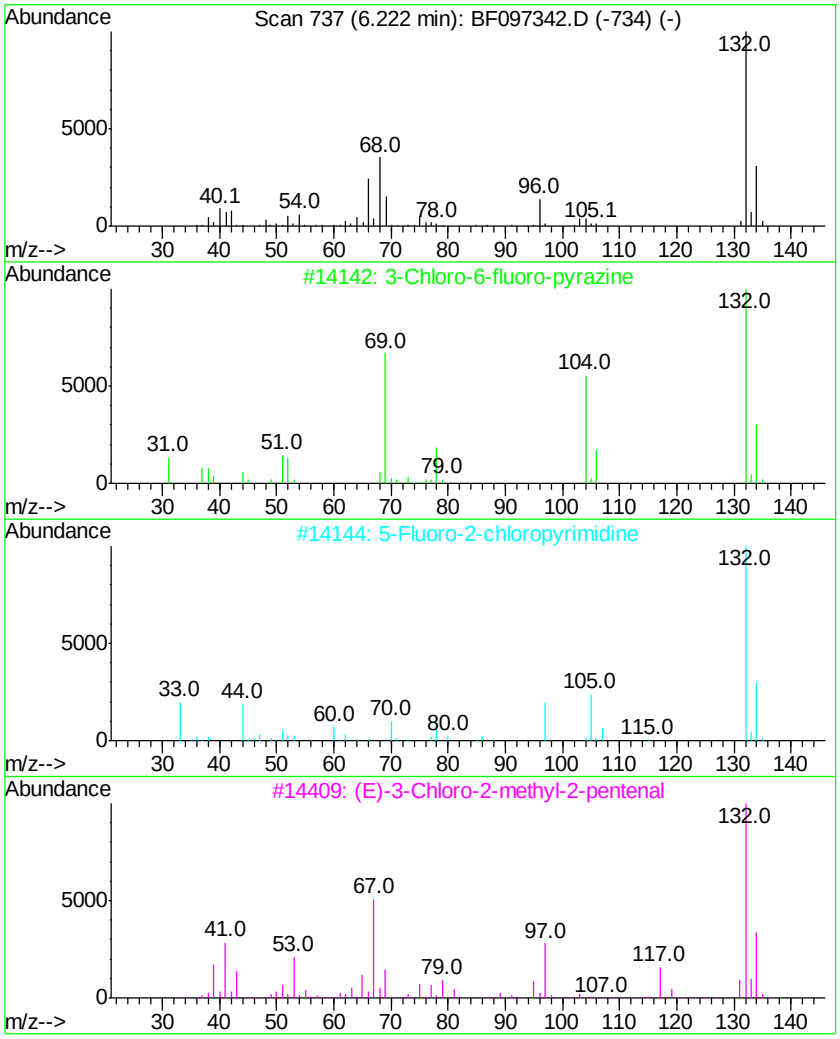
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

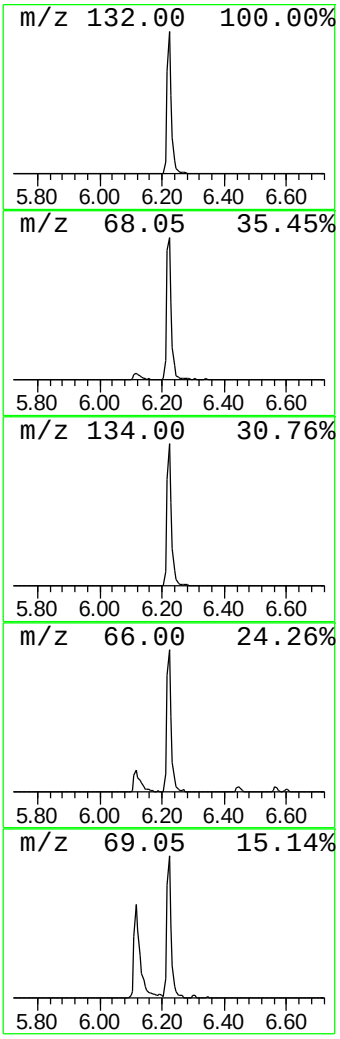
****

Peak Number 1 unknown6.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	16.81 ng	498724	1,4-Dichlorobenzene-d4	6.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	12





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Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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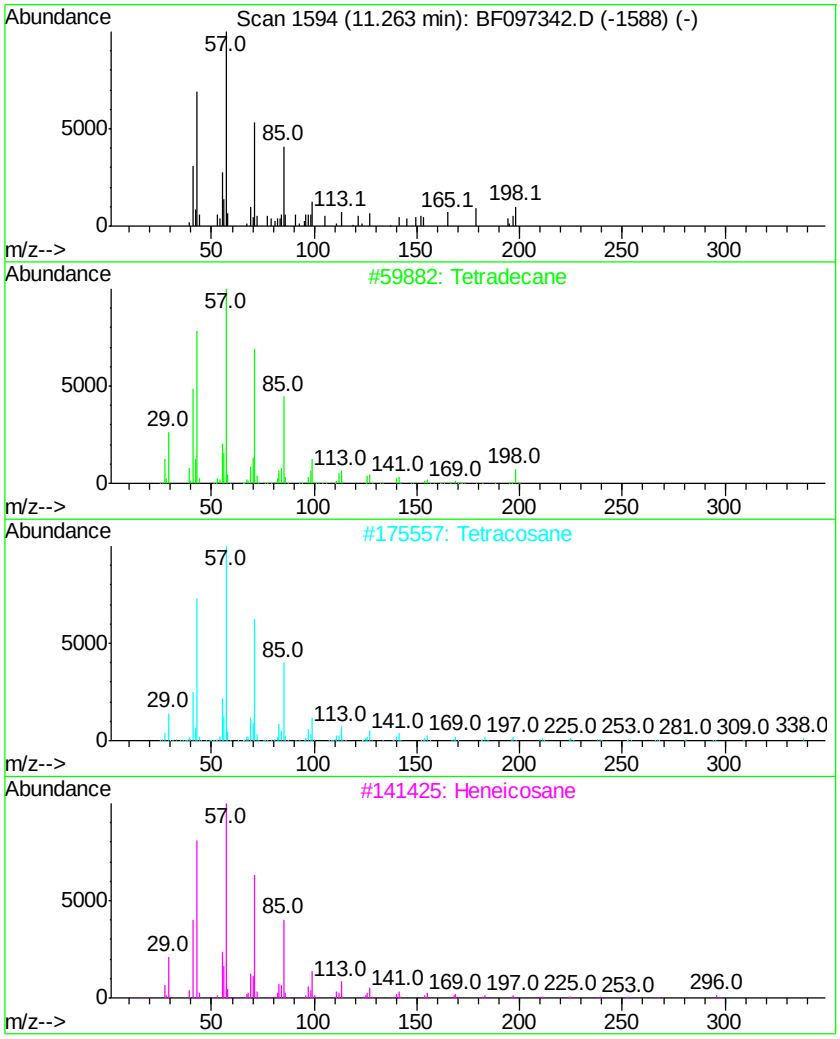
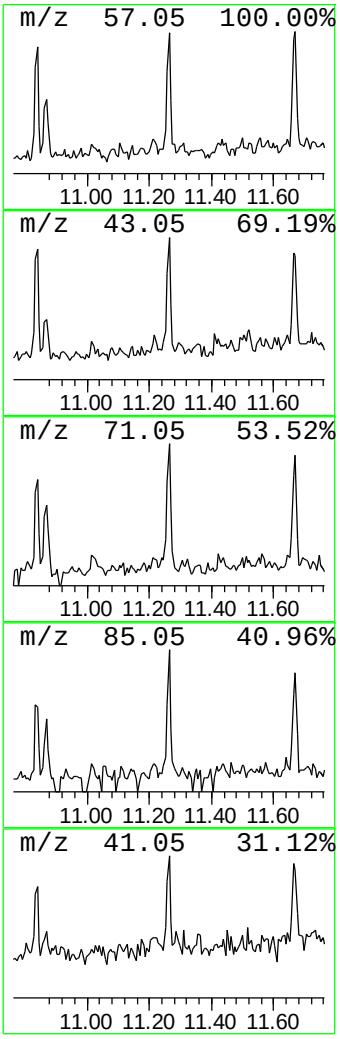
Peak Number 3 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.10 ng	55253	Phenanthrene-d10	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Tetracosane	338	C24H50	000646-31-1	68
3	Heneicosane	296	C21H44	000629-94-7	62
4	Octadecane	254	C18H38	000593-45-3	62
5	Octacosane	394	C28H58	000630-02-4	59





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Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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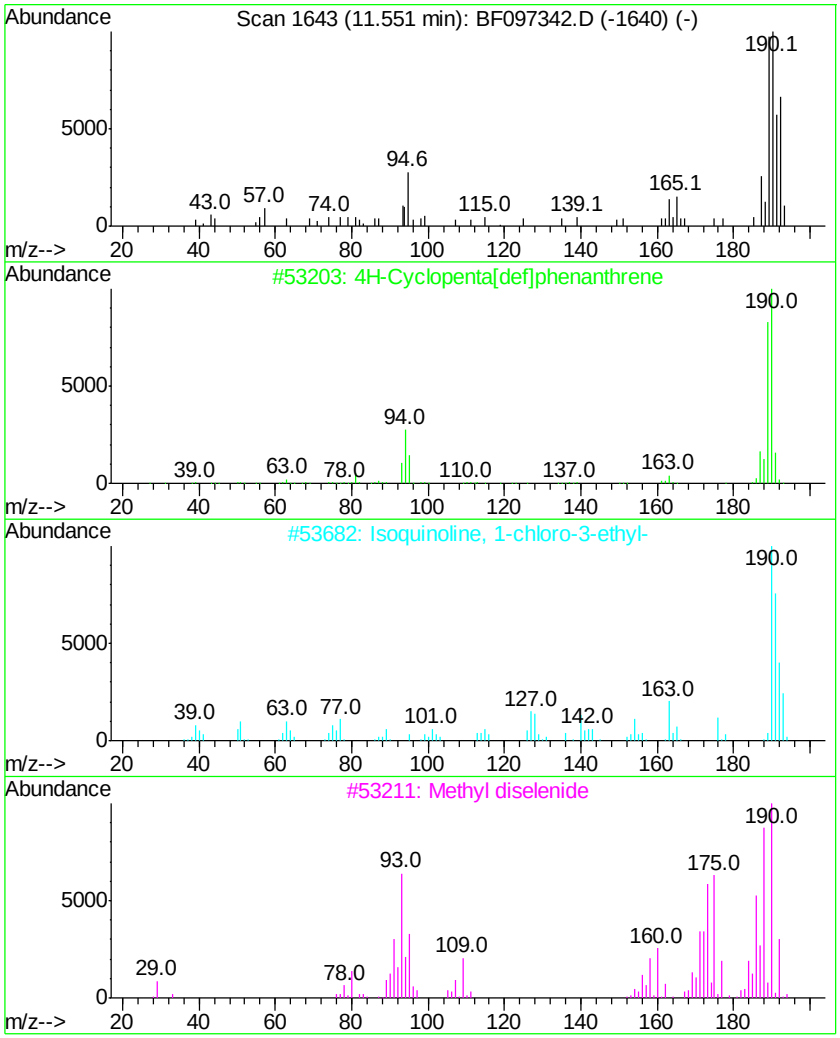
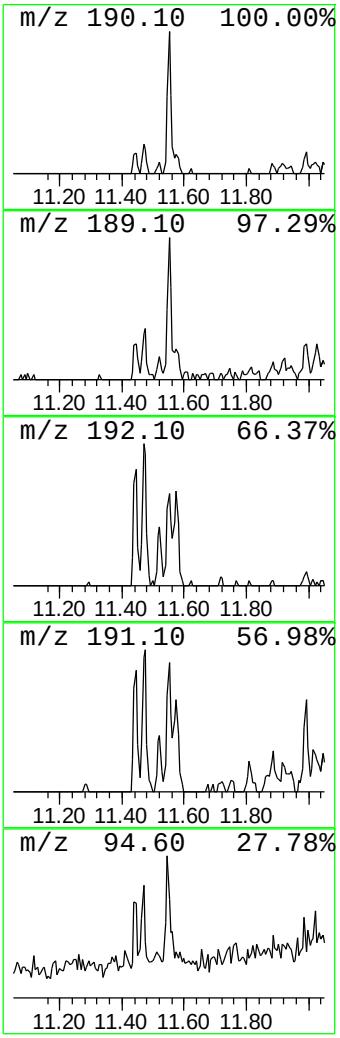
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.12 ng	55762	Phenanthrene-d10	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
2	Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	38
3	Methyl diselenide	190	C2H6Se2	007101-31-7	30
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	25
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	25





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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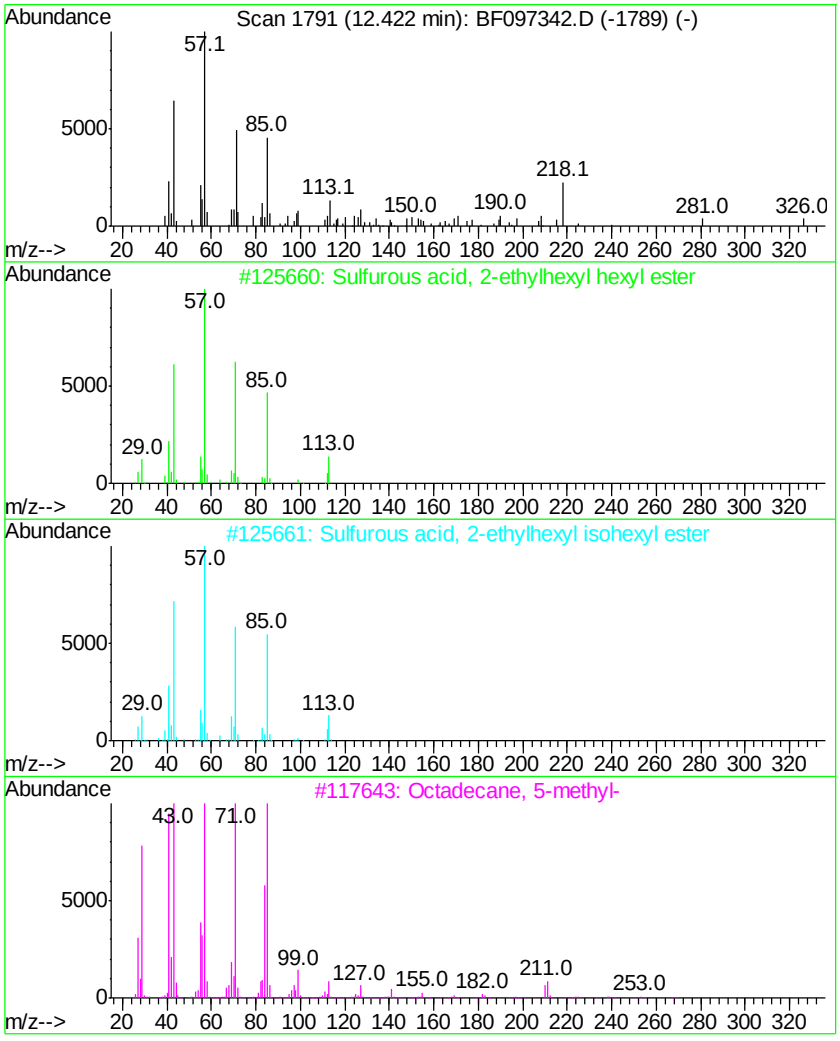
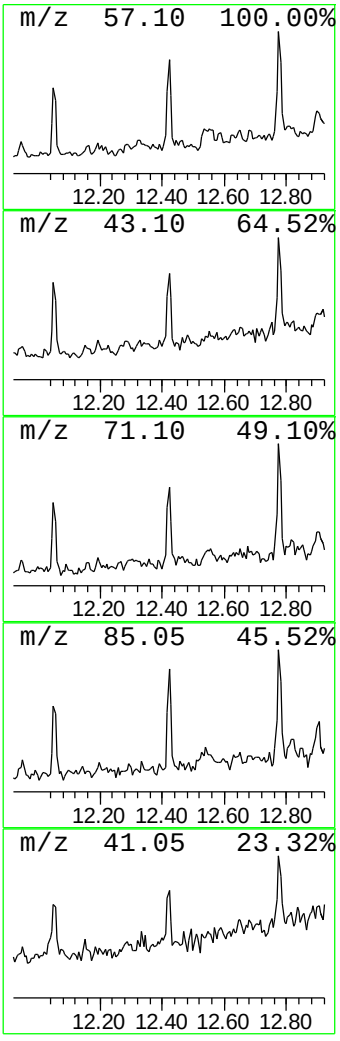
Peak Number 5 Sulfurous acid, 2-ethylhexy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	2.33 ng	61952	Chrysene-d12	13.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
2	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53
3	Octadecane, 5-methyl-	268	C19H40	025117-35-5	43
4	Hexadecane	226	C16H34	000544-76-3	38
5	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	38





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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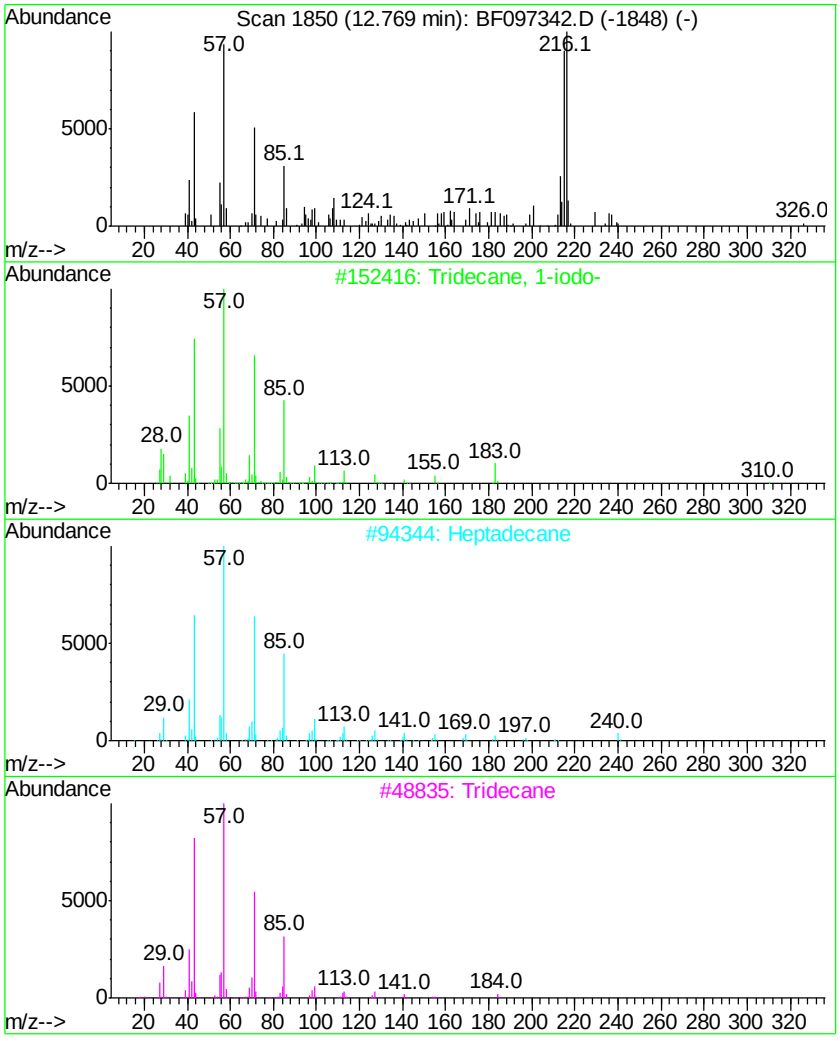
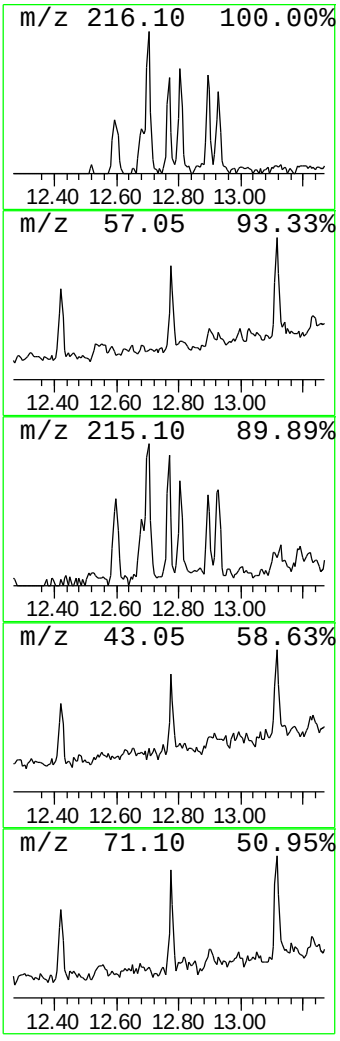
Peak Number 6 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.04 ng	54162	Chrysene-d12	13.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
2	Heptadecane	240	C17H36	000629-78-7	64
3	Tridecane	184	C13H28	000629-50-5	64
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	59
5	Docosane	310	C22H46	000629-97-0	59





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Data File : BF097342.D
Acq On : 4 Aug 2017 3:08
Operator : SJ/JU
Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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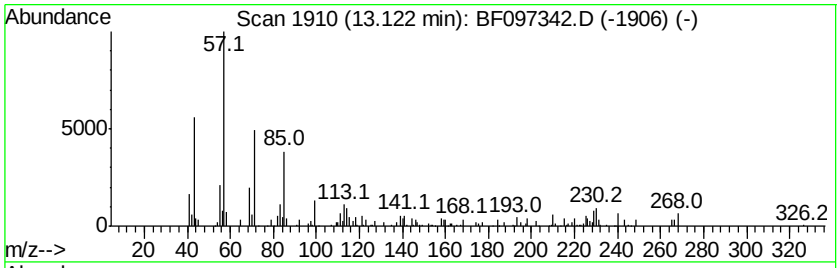
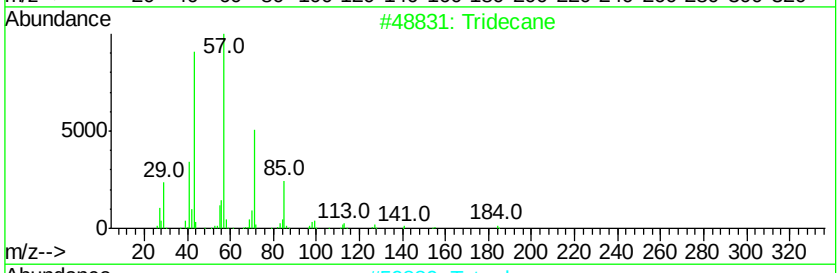
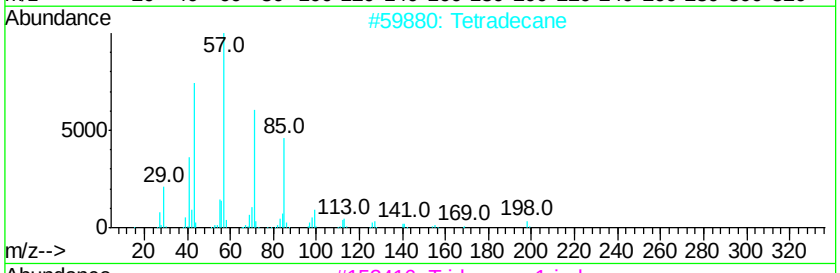
Peak Number 7 Tridecane Concentration Rank 5

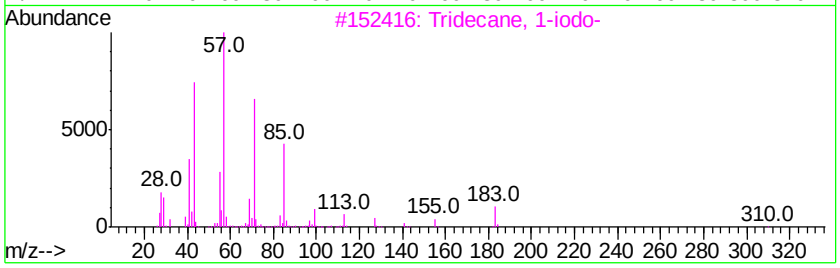
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	2.80 ng	74445	Chrysene-d12	13.56

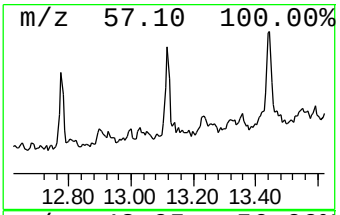
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	83
2	Tetradecane	198	C14H30	000629-59-4	83
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4	Eicosane	282	C20H42	000112-95-8	72
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	59

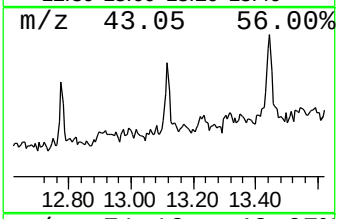


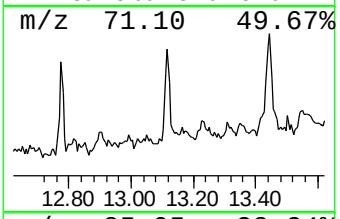


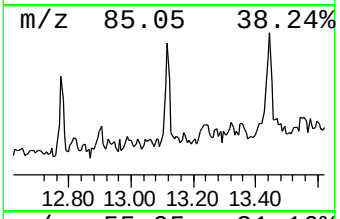


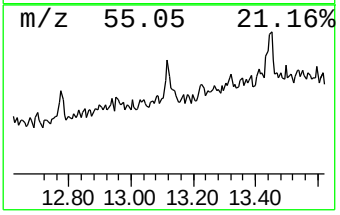












Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097342.D
Acq On : 4 Aug 2017 3:08
Operator : SJ/JU
Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

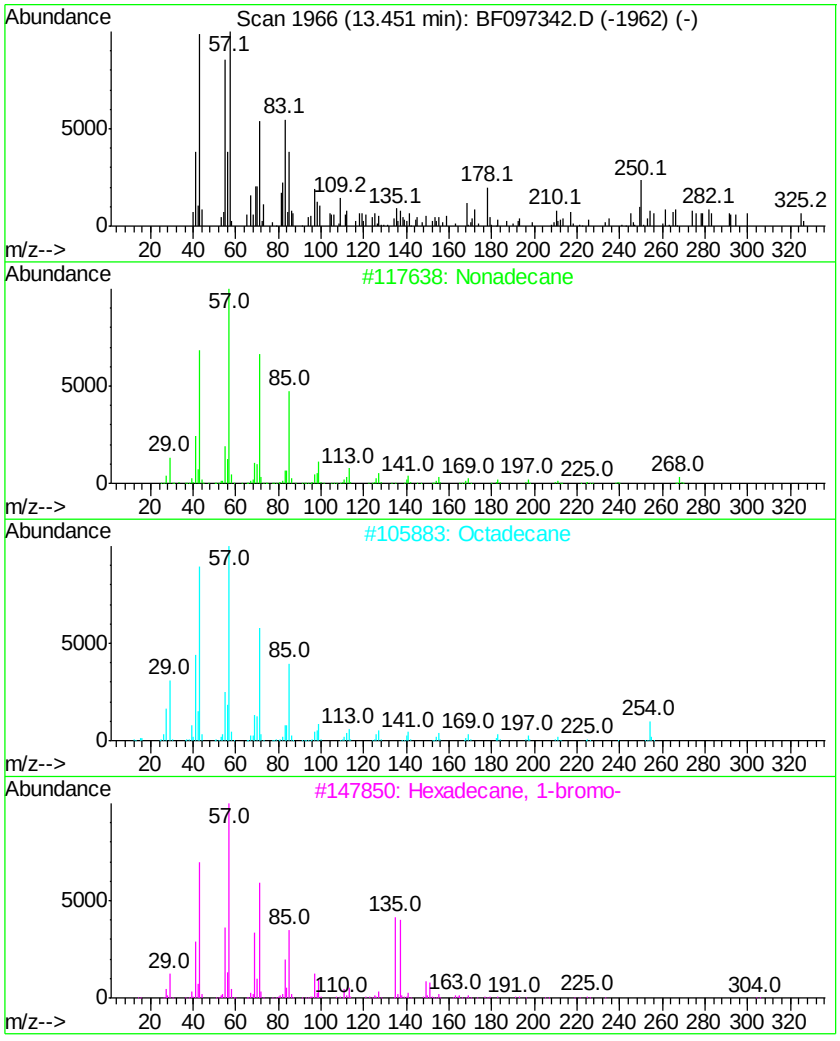
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

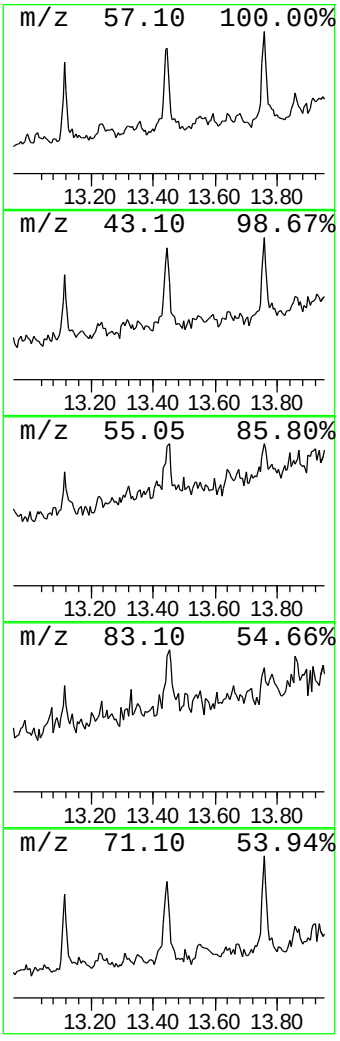
****

Peak Number 8 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	3.52 ng	93678	Chrysene-d12	13.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	83
2	Octadecane	254	C18H38	000593-45-3	83
3	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	74
4	Tetratetracontane	619	C44H90	007098-22-8	74
5	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	74





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097342.D
Acq On : 4 Aug 2017 3:08
Operator : SJ/JU
Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

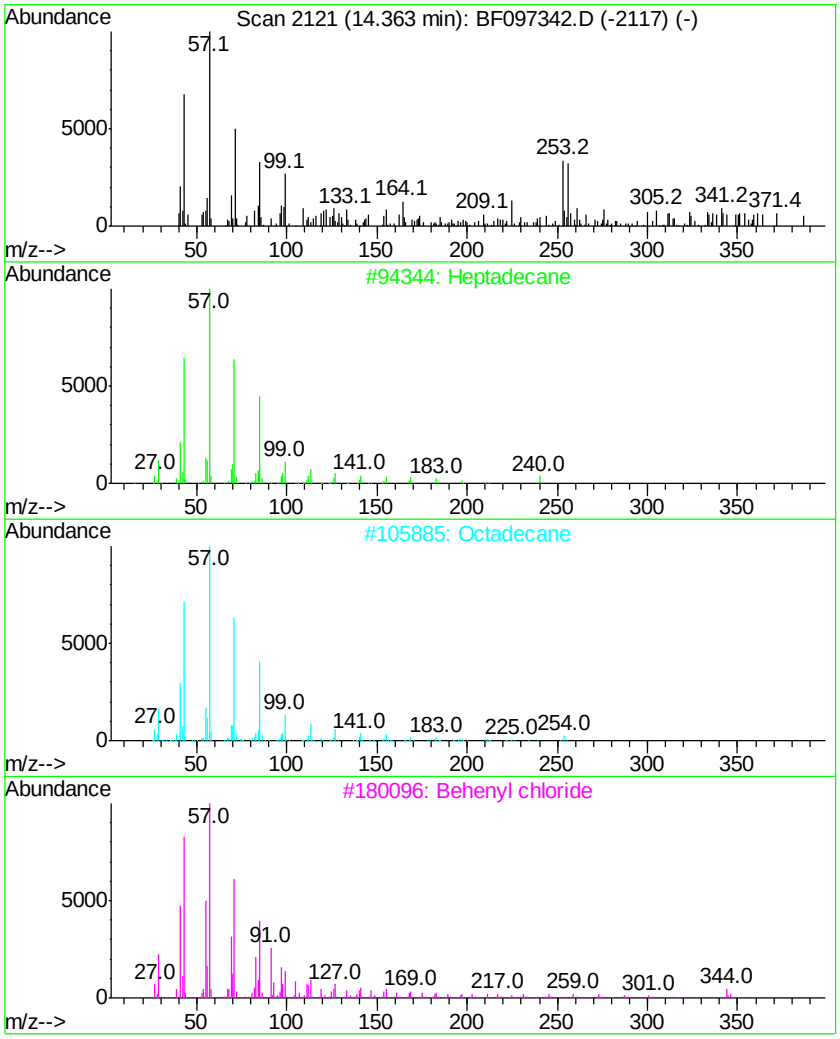
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

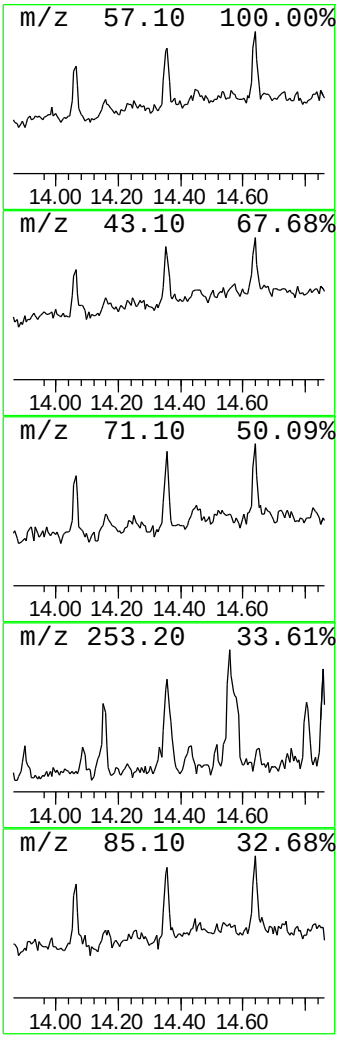
****

Peak Number 9 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	6.56 ng	88923	Perylene-d12	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Behenyl chloride	344	C22H45Cl	042217-03-8	76
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	68
5	Tetradecane	198	C14H30	000629-59-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097342.D
Acq On : 4 Aug 2017 3:08
Operator : SJ/JU
Sample : I4562-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-02-080117-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
unknown6.22	6.22	16.8	ng	498724	1	6.45	593431	20.0
Tetradecane	11.26	2.1	ng	55253	4	10.94	525873	20.0
4H-Cyclopenta[def...	11.55	2.1	ng	55762	4	10.94	525873	20.0
Sulfurous acid, 2...	12.42	2.3	ng	61952	5	13.56	532104	20.0
Tridecane, 1-iodo-	12.77	2.0	ng	54162	5	13.56	532104	20.0
Tridecane	13.12	2.8	ng	74445	5	13.56	532104	20.0
Nonadecane	13.45	3.5	ng	93678	5	13.56	532104	20.0
Heptadecane	14.36	6.6	ng	88923	6	14.91	271079	20.0