LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

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-BF081517.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	4.928	480	483	491	rVB	60059	64219	5.08%	0.408%
2	5.346	550	554	564	rVB	747073	695893	55.07%	4.421%
3	6.375	726	729	735	rBV	911740	779658	61.70%	4.953%
4	6.434	736	739	744	rVB2	13584	15487	1.23%	0.098%
5	6.510	749	752	756	rVV	786775	733910	58.08%	4.662%
6	6.587	760	765	767	rBV4	15810	17212	1.36%	0.109%
7	6.745	789	792	796	rBV	914177	834040	66.00%	5.298%
8	6.904	815	819	822	rBV	735629	592147	46.86%	3.762%
9	7.287	878	884	885	rBV	34610	34577	2.74%	0.220%
10	7.310	885	888	893	rVV	475810	439419	34.77%	2.791%
11	7.351	893	895	898	rVV2	28275	22811	1.81%	0.145%
12	7.398	898	903	906	rVB4	13525	16675	1.32%	0.106%
13	7.522	918	924	926	rBV2	22186	22210	1.76%	0.141%
14	7.545	926	928	933	rVB2	24206	27859	2.20%	0.177%
15	7.769	960	966	970	rBV2	45987	52471	4.15%	0.333%
16	8.034	1005	1011	1014	rBV	1192721	1047671	82.90%	6.655%
17	8.328	1053	1061	1063	rBV5	14051	23958	1.90%	0.152%
18	8.416	1073	1076	1079	rVB	21101	16012	1.27%	0.102%
19	8.457	1079	1083	1085	rBV	18240	17130	1.36%	0.109%
20	8.539	1092	1097	1100	rBV5	12362	15181	1.20%	0.096%
21	8.628	1108	1112	1115	rBV2	52372	44090	3.49%	0.280%
22	8.745	1130	1132	1135	rVB	18763	15548	1.23%	0.099%
23	8.839	1145	1148	1152	rBV2	28435	33928	2.68%	0.216%
24	9.057	1182	1185	1189	rVB2	28572	24909	1.97%	0.158%
25	9.104	1189	1193	1197	rBV	990955	838080	66.32%	5.324%
26	9.192	1204	1208	1213	rBV	70289	62396	4.94%	0.396%
27	9.369	1234	1238	1242	rBV5	17236	29926	2.37%	0.190%
28	9.445	1248	1251	1253	rBV2	25305	22760	1.80%	0.145%
29	9.469	1253	1255	1257	rVV2	25610	18989	1.50%	0.121%
30	9.504	1257	1261	1265	rVV2	98003	127855	10.12%	0.812%
31	9.563	1268	1271	1276	rVB5	14778	21501	1.70%	0.137%
32	9.645	1281	1285	1289	rBV	30688	39777	3.15%	0.253%
33	9.698	1290	1294	1296	rBV3	19796	22631	1.79%	0.144%
34	9.722	1296	1298	1302	rVB	86558	66132	5.23%	0.420%

LSC Area Percent Report

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Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.786	1302	1309	1312	rBV	992787	929344	73.54%	5.904%
36	9.892	1323	1327	1331	rVB4	19457	26563	2.10%	0.169%
37	9.986	1340	1343	1345	rVB	22112	22128	1.75%	0.141%
38	10.045	1351	1353	1356	rVB3	22098	20427	1.62%	0.130%
39	10.098	1360	1362	1365	rBV3	19914	23484	1.86%	0.149%
40	10.192	1375	1378	1380	rBV3	18716	19985	1.58%	0.127%
41	10.222	1380	1383	1386	rVB	97837	73005	5.78%	0.464%
42	10.328	1398	1401	1403	rBV3	24264	24568	1.94%	0.156%
43	10.392	1408	1412	1414	rVB5	13198	14722	1.16%	0.094%
44	10.439	1417	1420	1423	rVB	50752	48004	3.80%	0.305%
45	10.528	1432	1435	1437	rBV4	16562	17376	1.37%	0.110%
46	10.569	1438	1442	1446	rVV	370381	327717	25.93%	2.082%
47	10.663	1454	1458	1460	rBV5	12221	18834	1.49%	0.120%
48	10.692	1460	1463	1472	rVV2	139523	194955	15.43%	1.238%
49	10.904	1497	1499	1505	rVB5	26671	34087	2.70%	0.217%
50	11.139	1537	1539	1541	rBV	94619	71503	5.66%	0.454%
51	11.169	1541	1544	1549	rVB2	72067	84391	6.68%	0.536%
52	11.269	1557	1561	1563	rBV	814997	772247	61.11%	4.906%
53	11.286	1563	1564	1568	rVV	126475	86686	6.86%	0.551%
54	11.339	1571	1573	1576	rVB	41855	34452	2.73%	0.219%
55	11.380	1577	1580	1582	rBV3	15607	21117	1.67%	0.134%
56	11.522	1602	1604	1606	rVB	22841	18010	1.43%	0.114%
57	11.569	1609	1612	1614	rBV	74186	65286	5.17%	0.415%
58	11.669	1625	1629	1634	rVB	414564	357014	28.25%	2.268%
59	11.769	1643	1646	1648	rBV	50140	43539	3.45%	0.277%
60	11.792	1648	1650	1654	rVB	68464	58521	4.63%	0.372%
61	11.839	1655	1658	1660	rBV3	23282	24033	1.90%	0.153%
62	11.875	1661	1664	1667	rBV	95032	103306	8.17%	0.656%
63	11.975	1678	1681	1683	rBV	58262	48983	3.88%	0.311%
64	11.998	1683	1685	1688	rVB3	18687	17641	1.40%	0.112%
65	12.063	1693	1696	1698	rBV2	28967	28429	2.25%	0.181%
66	12.192	1716	1718	1720	rBV2	17099	17241	1.36%	0.110%
67	12.245	1724	1727	1733	rBV4	26943	48403	3.83%	0.307%
68	12.316	1736	1739	1741	rVV	67683	63695	5.04%	0.405%
69	12.351	1741	1745	1747	rVV	1446203	1263711	100.00%	8.028%
70	12.374	1747	1749	1751	rVV	1091261	859753	68.03%	5.462%
71	12.392	1751	1752	1758	rVV4	100010	93658	7.41%	0.595%

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Misc :
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Instrument : BNA_F
ClientSampleId : SU-04-082117

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.457	1760	1763	1764	rVV	184140	149629	11.84%	0.951%
73	12.474	1764	1766	1769	rVB	238907	193456	15.31%	1.229%
74	12.704	1800	1805	1808	rBV	286835	298101	23.59%	1.894%
75	12.733	1808	1810	1812	rVB2	51447	39747	3.15%	0.252%
76	12.851	1826	1830	1835	rVB	672542	631548	49.98%	4.012%
77	12.922	1840	1842	1850	rVV3	29247	57598	4.56%	0.366%
78	13.092	1868	1871	1875	rVB3	78458	87727	6.94%	0.557%
79	13.133	1875	1878	1881	rBV	58463	62961	4.98%	0.400%
80	13.257	1896	1899	1903	rBV	46763	45119	3.57%	0.287%
81	13.433	1926	1929	1931	rBV2	59082	57622	4.56%	0.366%
82	13.898	2004	2008	2011	rBV	838547	883052	69.88%	5.610%
83	15.321	2247	2250	2255	rBV	353430	421480	33.35%	2.677%

Sum of corrected areas: 15741920

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Operator : SJ/JU
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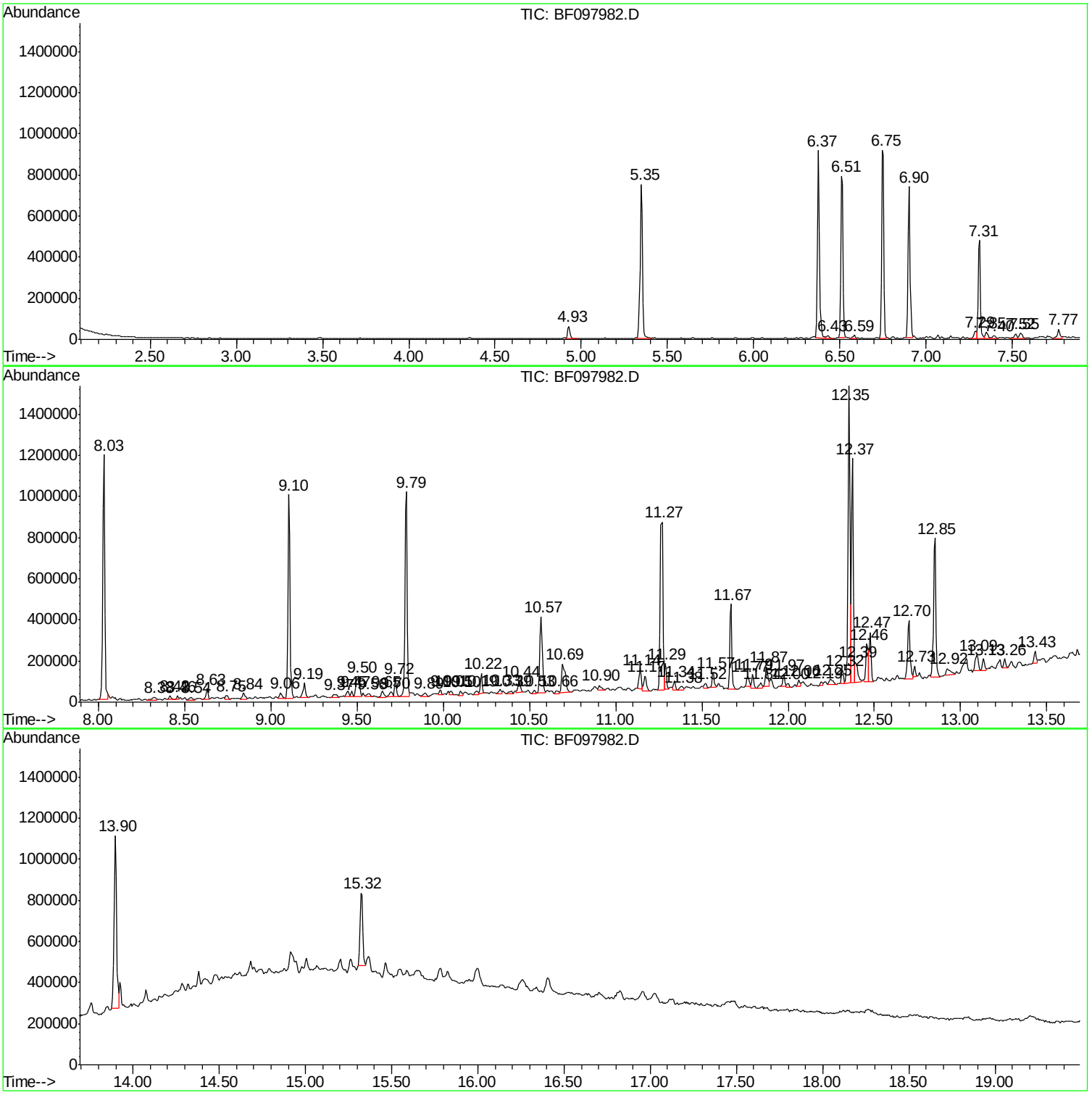
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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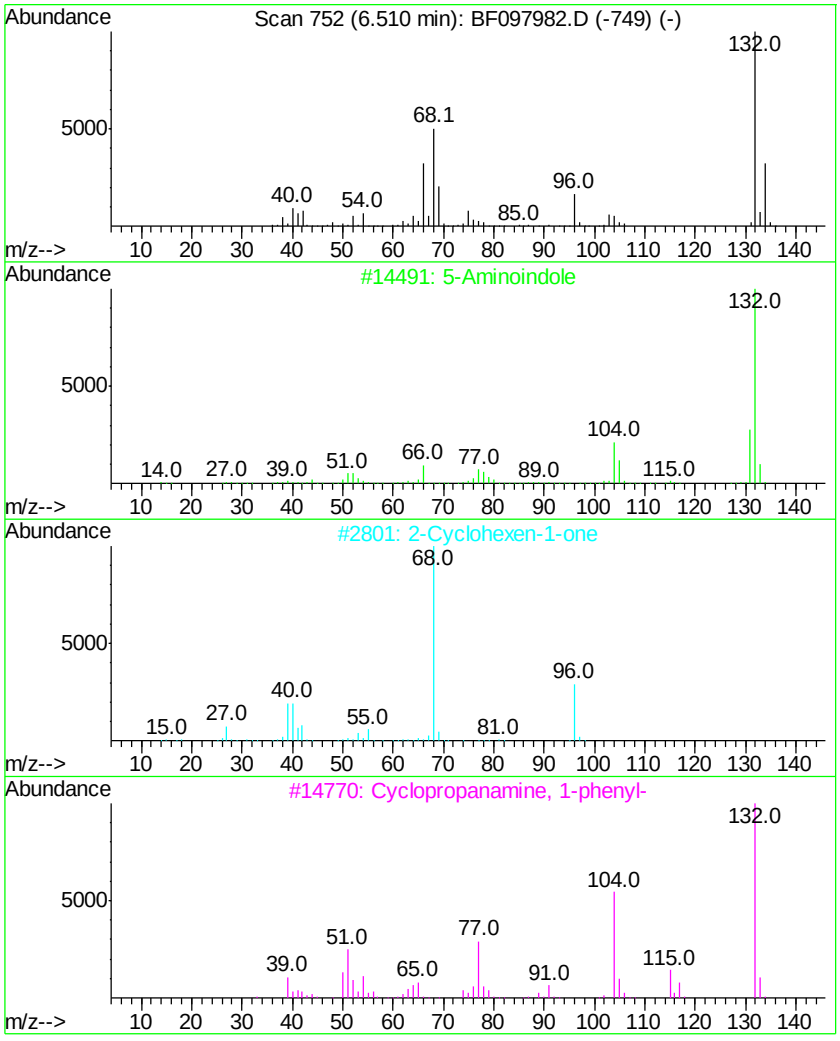
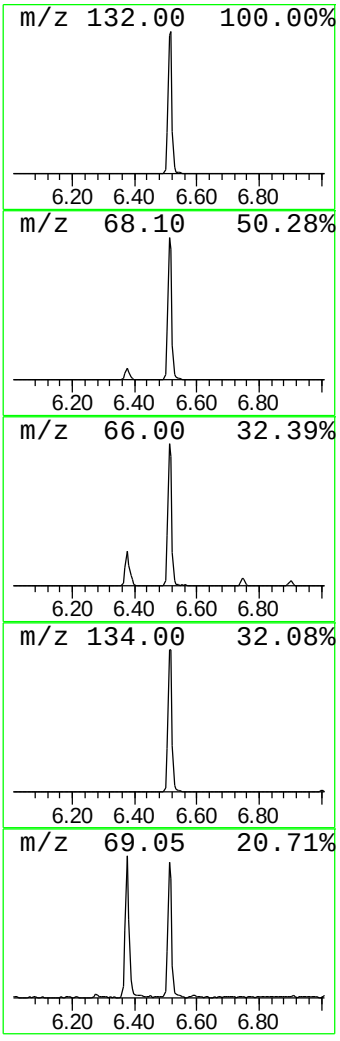
Peak Number 1 unknown6.51 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	17.60 ng	733910	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Aminoindan	133	C9H11N	034698-41-4	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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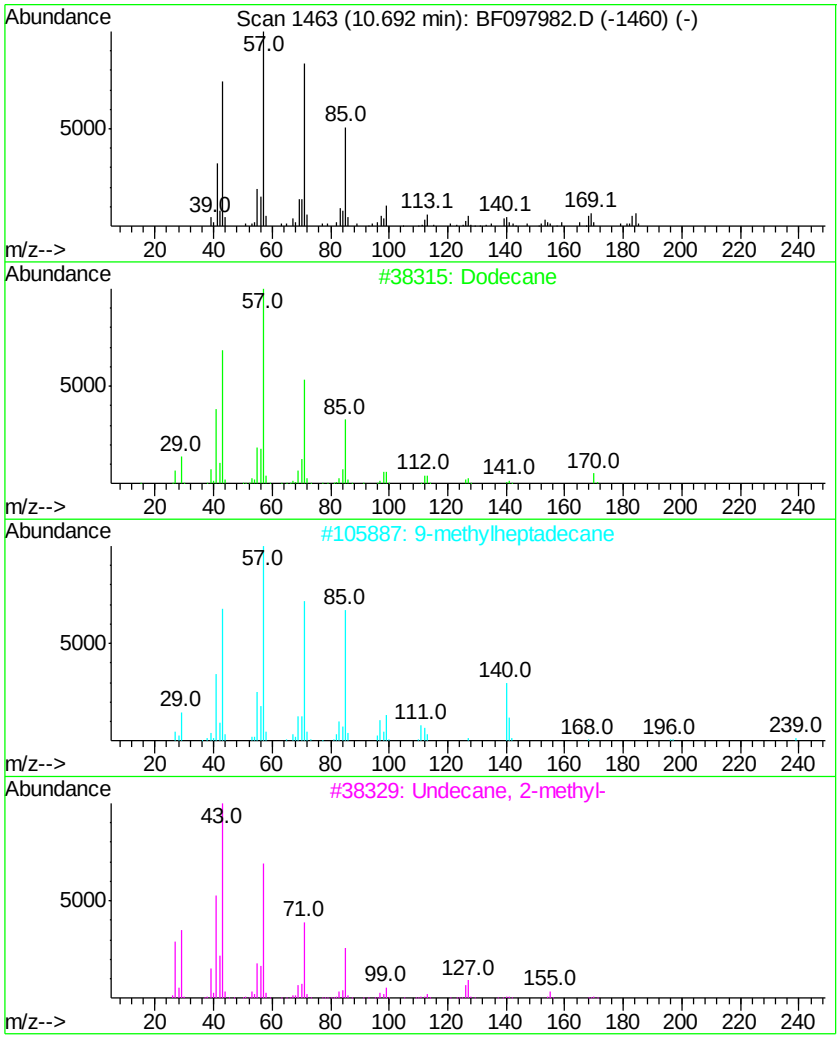
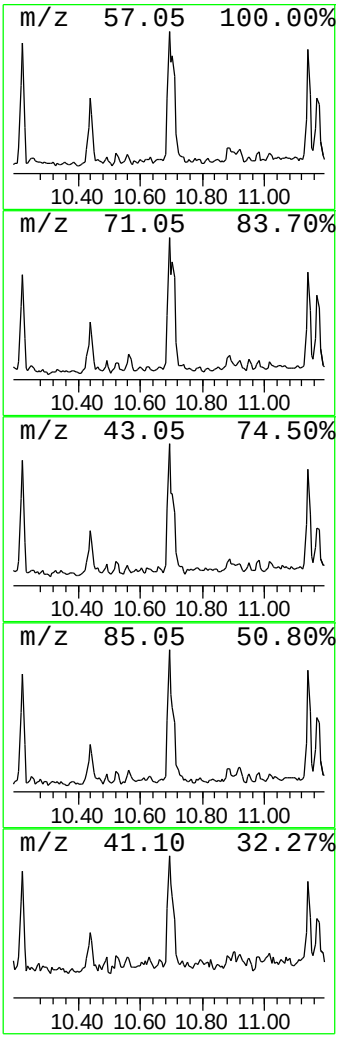
Peak Number 3 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	5.05 ng	194955	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	87
2	9-methylheptadecane	254	C18H38	026741-18-4	83
3	Undecane, 2-methyl-	170	C12H26	007045-71-8	80
4	Tridecane	184	C13H28	000629-50-5	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
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Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

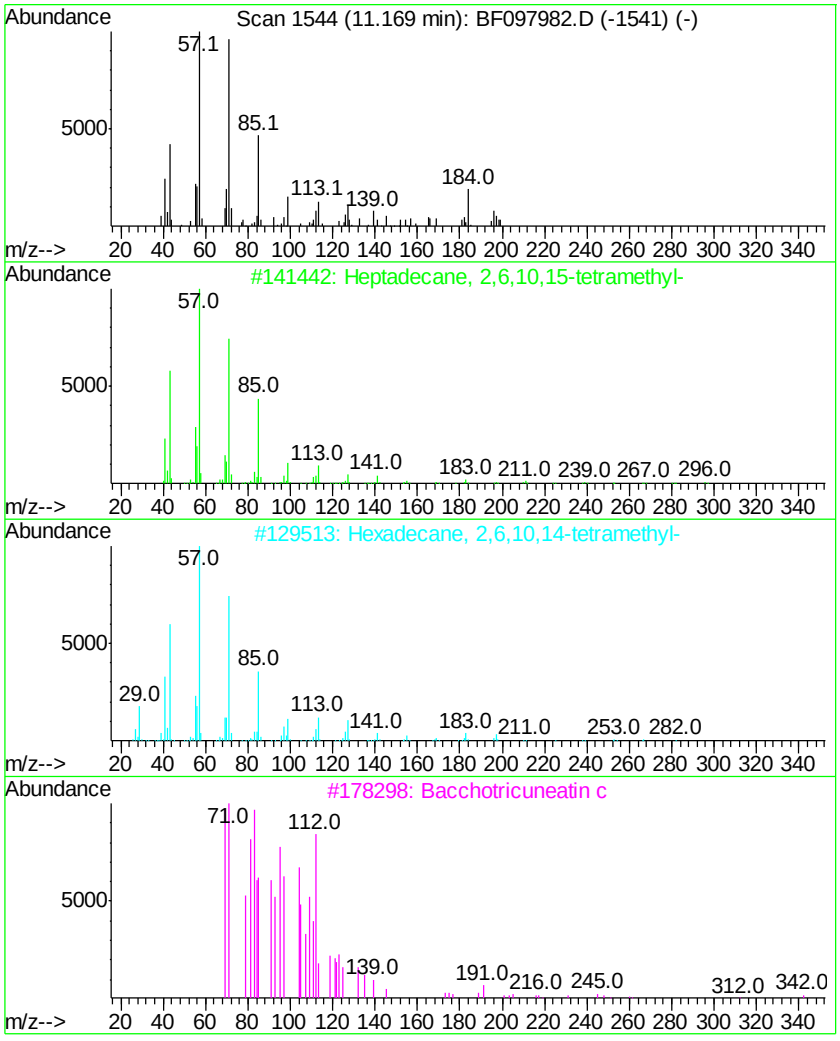
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

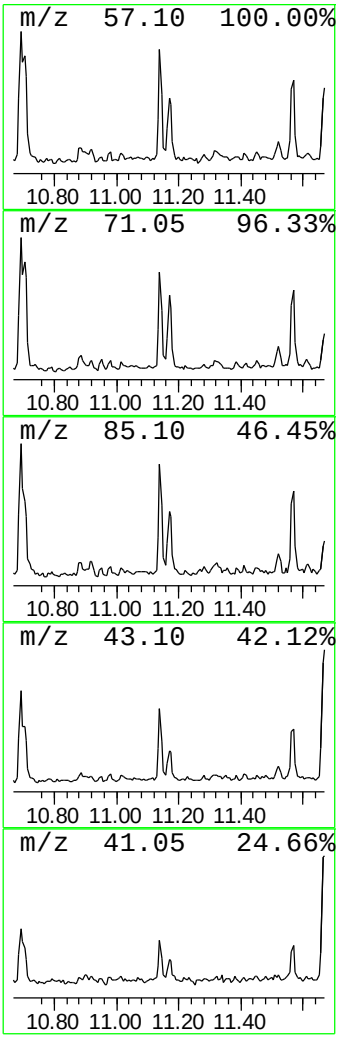
****

Peak Number 4 Heptadecane, 2,6,10,15-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	2.19 ng	84391	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
3	Bacchotricuneatin c	342	C20H22O5	066563-30-2	53
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	50
5	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	50





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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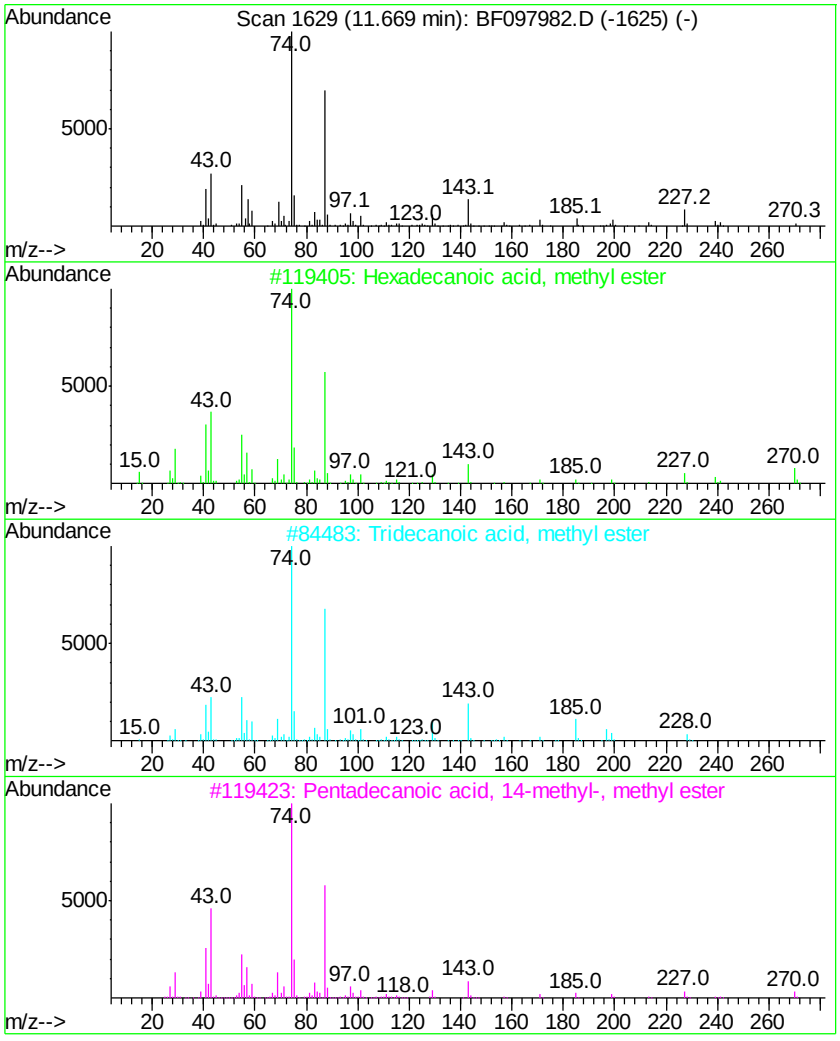
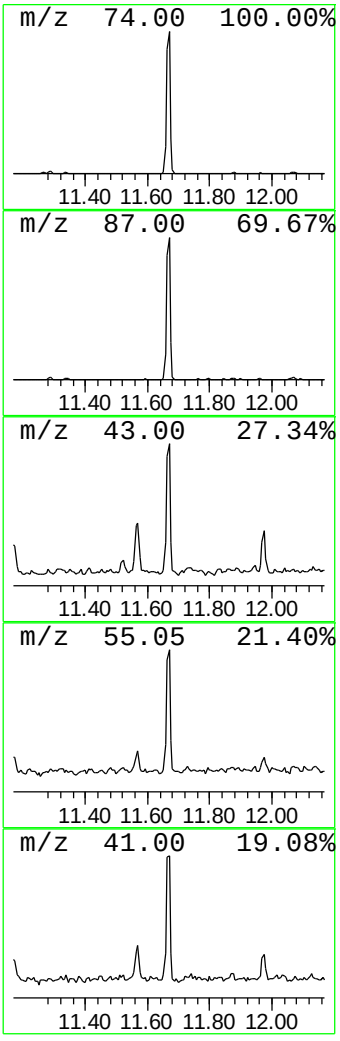
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	9.25 ng	357014	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	94
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

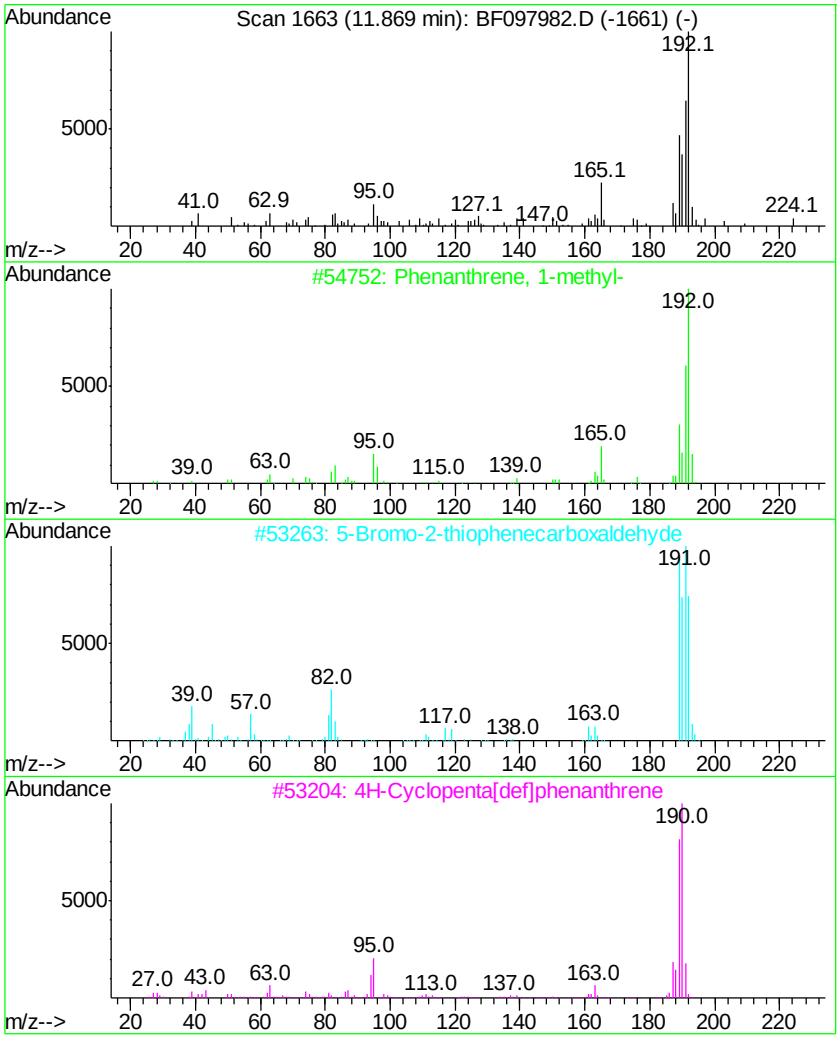
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

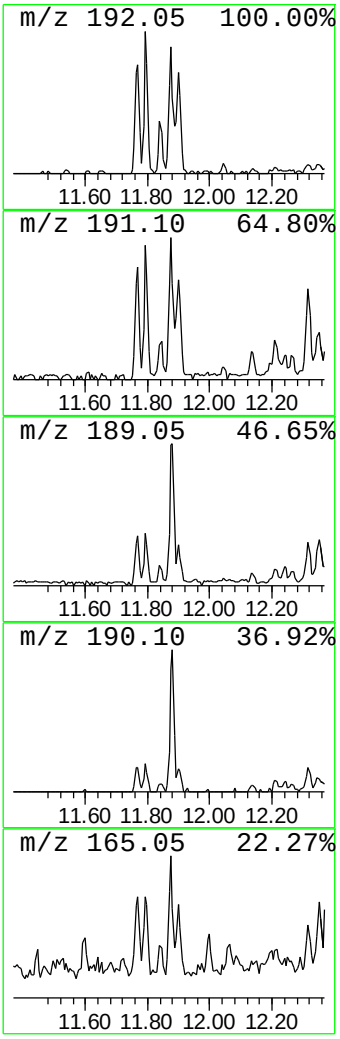
****

Peak Number 6 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.68 ng	103306	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	62
2	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	58
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
4	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	41
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	41





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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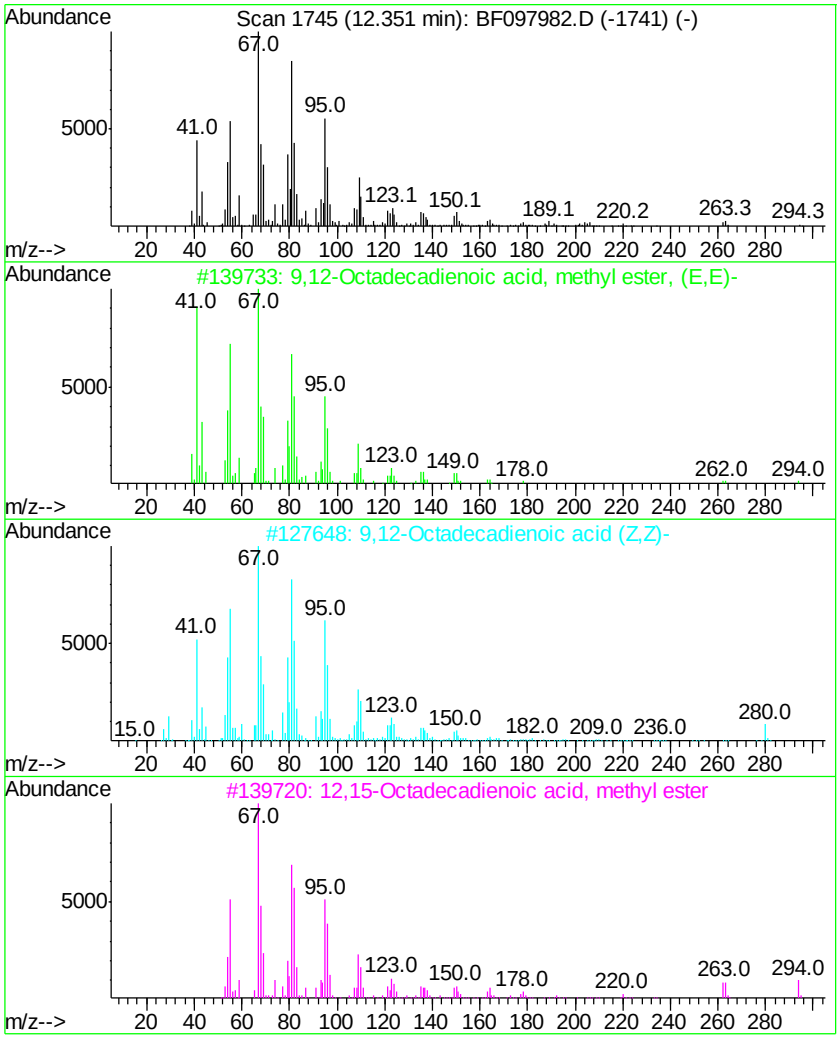
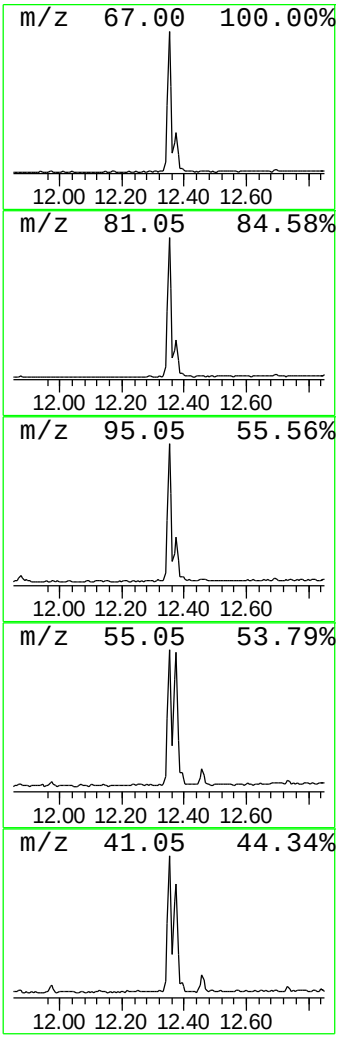
Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	32.73 ng	1263710	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
3	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	91
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	90
5	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	90





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Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

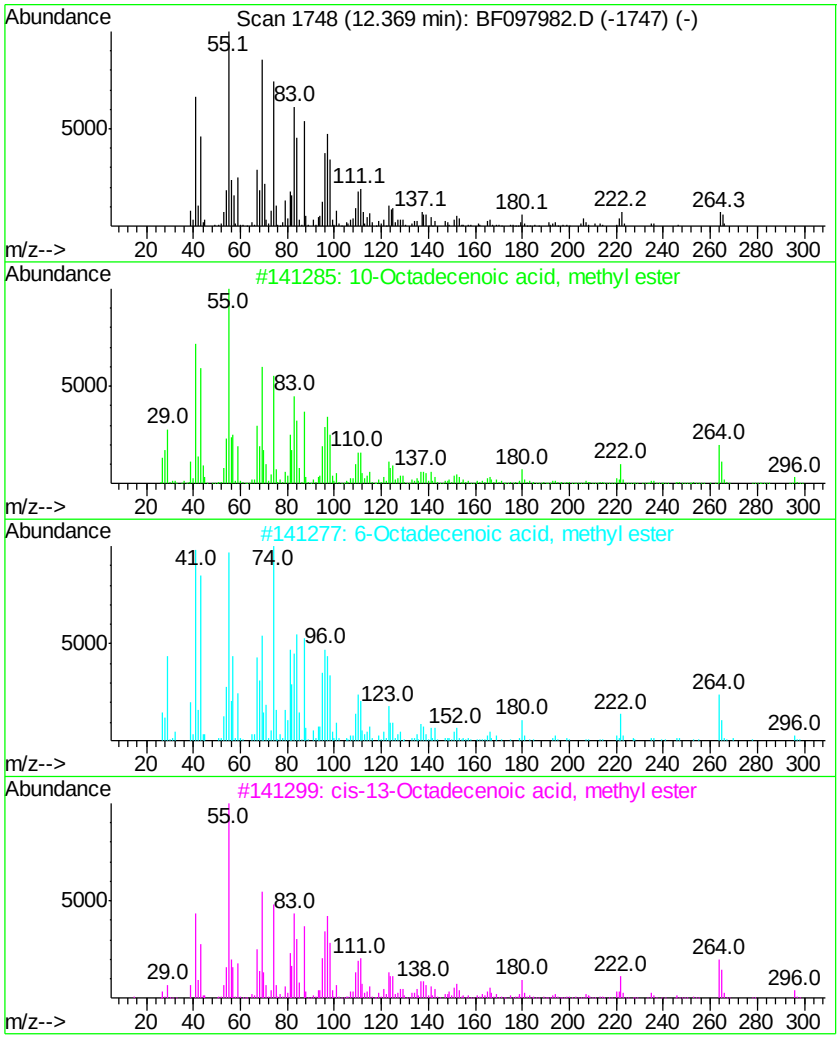
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

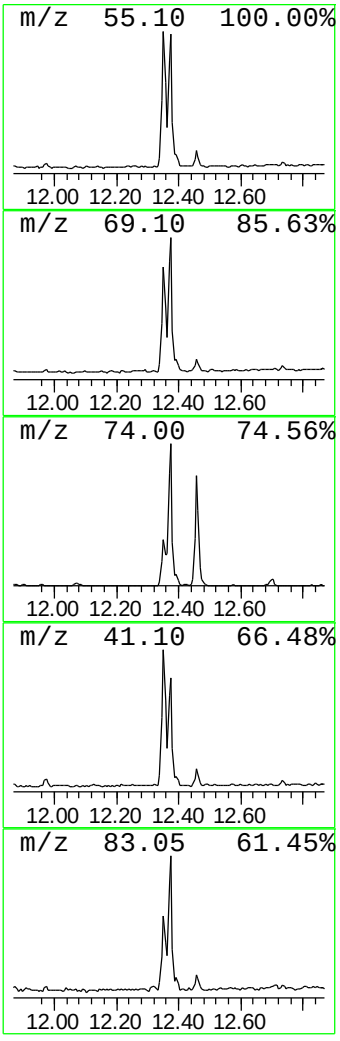
****

Peak Number 8 10-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	22.27 ng	859753	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
2	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
3	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	95
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	95
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

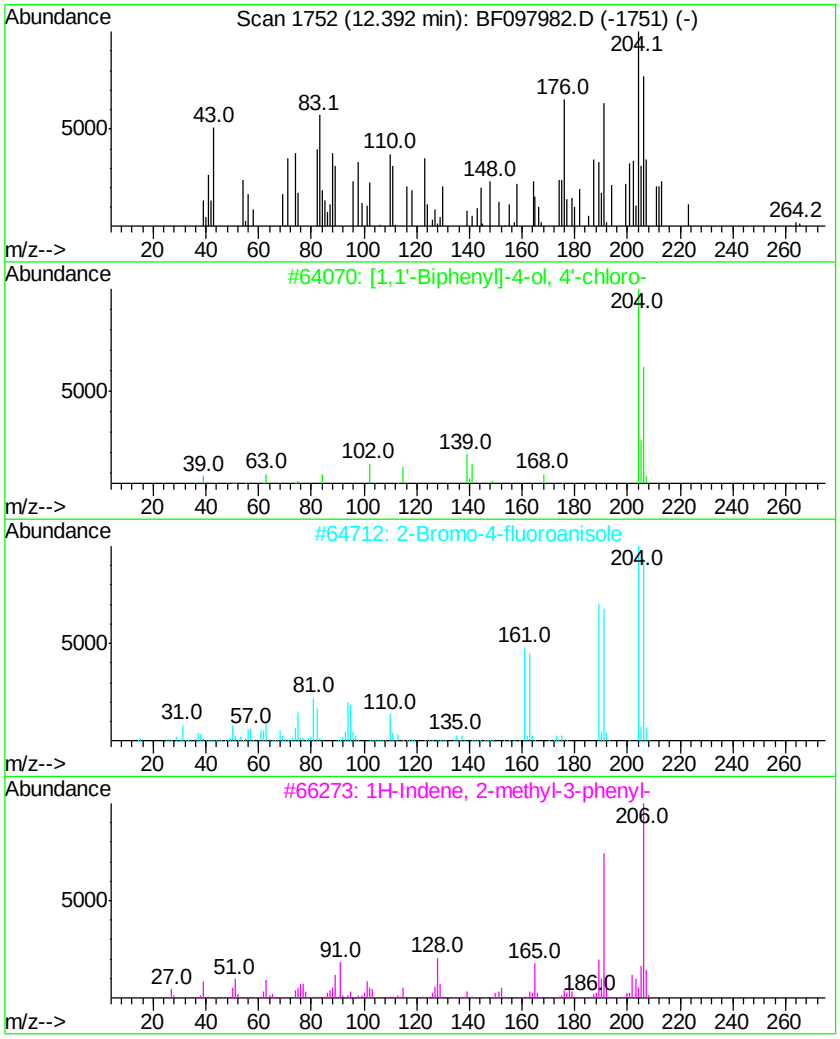
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

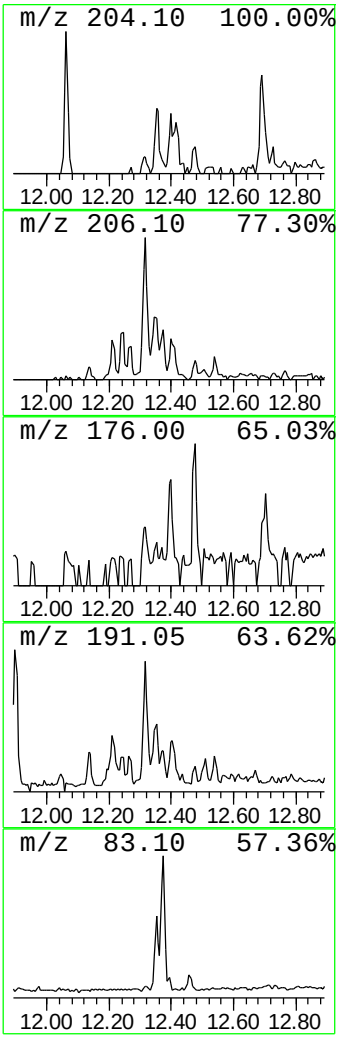
****

Peak Number 9 unknown12.39 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	2.43 ng	93658	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,1'-Biphenyl]-4-ol, 4'-chloro-	204	C12H9ClO	028034-99-3	38
2	2-Bromo-4-fluoroanisole	204	C7H6BrFO	000452-08-4	38
3	1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	27
4	9,10-Dimethylanthracene	206	C16H14	000781-43-1	27
5	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	27





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF082217\
Data File : BF097982.D
Acq On : 23 Aug 2017 4:39
Operator : SJ/JU
Sample : I4909-01 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-04-082117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
unknown6.51	6.51	17.6	ng	733910	1	6.75	834040	20.0
Dodecane	10.69	5.0	ng	194955	4	11.27	772247	20.0
Heptadecane, 2,6,...	11.17	2.2	ng	84391	4	11.27	772247	20.0
Hexadecanoic acid...	11.67	9.3	ng	357014	4	11.27	772247	20.0
Phenanthrene, 1-m...	11.87	2.7	ng	103306	4	11.27	772247	20.0
9,12-Octadecadien...	12.35	32.7	ng	1263710	4	11.27	772247	20.0
10-Octadecenoic a...	12.37	22.3	ng	859753	4	11.27	772247	20.0
unknown12.39	12.39	2.4	ng	93658	4	11.27	772247	20.0