LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030419\
Data File : BF112822.D
Acq On : 4 Mar 2019 14:18
Operator : JU/SJ
Sample : K1707-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

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-BF022719.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	4.445	396	401	405	rBV	84505	97591	2.26%	0.202%
2	5.357	551	556	559	rBV	3859155	3867713	89.63%	7.995%
3	6.287	710	714	720	rVB4	42604	55857	1.29%	0.115%
4	6.381	725	730	733	rBV	3900254	4288984	99.40%	8.866%
5	6.516	748	753	756	rBV	4558722	4314965	100.00%	8.919%
6	6.745	788	792	795	rBV	1295857	1035910	24.01%	2.141%
7	6.904	815	819	822	rBV	3819067	3285953	76.15%	6.792%
8	7.069	844	847	850	rBV2	62079	60867	1.41%	0.126%
9	7.145	856	860	863	rBV2	64303	63057	1.46%	0.130%
10	7.304	879	887	890	rBV	2871909	2879128	66.72%	5.951%
11	7.528	919	925	929	rBV4	29045	56864	1.32%	0.118%
12	8.028	1006	1010	1012	rBV	1380265	1295045	30.01%	2.677%
13	8.045	1012	1013	1021	rVB	194377	178312	4.13%	0.369%
14	8.363	1064	1067	1073	rBV6	29636	59091	1.37%	0.122%
15	8.463	1082	1084	1087	rVB	74023	55559	1.29%	0.115%
16	8.633	1110	1113	1119	rVB	60105	51835	1.20%	0.107%
17	8.739	1125	1131	1135	rBV2	155758	153249	3.55%	0.317%
18	8.833	1144	1147	1151	rBV	64527	60377	1.40%	0.125%
19	9.104	1188	1193	1196	rBV	4448755	4229828	98.03%	8.743%
20	9.192	1206	1208	1212	rVB2	99550	100853	2.34%	0.208%
21	9.363	1234	1237	1243	rVB2	34221	51276	1.19%	0.106%
22	9.439	1247	1250	1252	rBV2	58000	58008	1.34%	0.120%
23	9.492	1256	1259	1261	rBV	276900	223678	5.18%	0.462%
24	9.633	1279	1283	1286	rBV	47237	49058	1.14%	0.101%
25	9.722	1295	1298	1302	rVB	93475	75679	1.75%	0.156%
26	9.775	1302	1307	1311	rBV	1685339	1508551	34.96%	3.118%
27	9.804	1311	1312	1317	rVB2	80778	70335	1.63%	0.145%
28	9.980	1339	1342	1345	rVB	94293	88371	2.05%	0.183%
29	10.092	1357	1361	1364	rBV3	39059	49334	1.14%	0.102%
30	10.186	1373	1377	1380	rBV3	46786	64046	1.48%	0.132%
31	10.222	1380	1383	1386	rVV	69995	58650	1.36%	0.121%
32	10.316	1397	1399	1401	rBV	56769	50232	1.16%	0.104%
33	10.439	1417	1420	1423	rBV3	41091	51333	1.19%	0.106%
34	10.557	1436	1440	1446	rBV	2823946	2836908	65.75%	5.864%

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Misc :
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Instrument : BNA_F
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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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.692	1460	1463	1464	rBV2	108840	96927	2.25%	0.200%
36	11.057	1523	1525	1530	rVB3	63797	65749	1.52%	0.136%
37	11.139	1537	1539	1542	rBV2	75138	68205	1.58%	0.141%
38	11.251	1555	1558	1561	rBV	1514718	1408795	32.65%	2.912%
39	11.274	1561	1562	1565	rVV	439326	277462	6.43%	0.574%
40	11.327	1569	1571	1574	rVB	104379	86760	2.01%	0.179%
41	11.757	1641	1644	1646	rBV	113129	112135	2.60%	0.232%
42	11.792	1646	1650	1653	rBV2	651969	686289	15.90%	1.419%
43	11.863	1659	1662	1665	rBV	209291	227983	5.28%	0.471%
44	11.968	1678	1680	1682	rBV	66773	52435	1.22%	0.108%
45	12.045	1691	1693	1695	rBV	112537	98658	2.29%	0.204%
46	12.304	1734	1737	1740	rBV	156522	153520	3.56%	0.317%
47	12.357	1744	1746	1748	rVB	111633	81488	1.89%	0.168%
48	12.386	1748	1751	1756	rVB4	76524	102142	2.37%	0.211%
49	12.463	1760	1764	1767	rBV	746822	722010	16.73%	1.492%
50	12.574	1780	1783	1787	rBV2	279857	290922	6.74%	0.601%
51	12.686	1797	1802	1805	rBV	876101	861403	19.96%	1.781%
52	12.839	1824	1828	1831	rBV	3123815	3073435	71.23%	6.353%
53	12.910	1837	1840	1843	rBV	84501	91063	2.11%	0.188%
54	13.015	1856	1858	1861	rVB2	169696	147628	3.42%	0.305%
55	13.080	1866	1869	1872	rVB	170676	144155	3.34%	0.298%
56	13.115	1873	1875	1878	rVV	118112	114596	2.66%	0.237%
57	13.210	1889	1891	1894	rVB	91001	68853	1.60%	0.142%
58	13.239	1894	1896	1899	rVB	93856	80808	1.87%	0.167%
59	13.421	1924	1927	1929	rBV	96780	87976	2.04%	0.182%
60	13.521	1941	1944	1949	rVB	114027	155478	3.60%	0.321%
61	13.627	1959	1962	1965	rBV2	112467	145483	3.37%	0.301%
62	13.680	1969	1971	1975	rVV2	72376	79397	1.84%	0.164%
63	13.739	1978	1981	1988	rVB2	400917	480821	11.14%	0.994%
64	13.880	2000	2005	2008	rBV2	1515970	1865112	43.22%	3.855%
65	13.904	2008	2009	2012	rVB	444732	276966	6.42%	0.573%
66	14.062	2034	2036	2039	rVB2	158515	129413	3.00%	0.268%
67	14.268	2069	2071	2074	rVB	140047	97626	2.26%	0.202%
68	14.298	2074	2076	2080	rVB	112877	95381	2.21%	0.197%
69	14.368	2085	2088	2090	rVV2	174847	161233	3.74%	0.333%
70	14.662	2135	2138	2144	rVB2	258255	312037	7.23%	0.645%
71	14.892	2173	2177	2184	rBV	449377	780867	18.10%	1.614%

LSC Area Percent Report

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Instrument : BNA_F
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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.986	2189	2193	2199	rVB3	293805	402445	9.33%	0.832%
73	15.174	2222	2225	2231	rVB	259752	290084	6.72%	0.600%
74	15.233	2231	2235	2240	rVB	346550	400258	9.28%	0.827%
75	15.292	2241	2245	2249	rVV	926425	1115982	25.86%	2.307%
76	15.345	2251	2254	2258	rVB	241715	291382	6.75%	0.602%
77	15.751	2319	2323	2327	rBV	193960	273374	6.34%	0.565%
78	16.221	2400	2403	2412	rVB2	111676	177140	4.11%	0.366%
79	16.656	2473	2477	2484	rVB2	126947	219437	5.09%	0.454%

Sum of corrected areas: 48377810

LSC Report - Integrated Chromatogram

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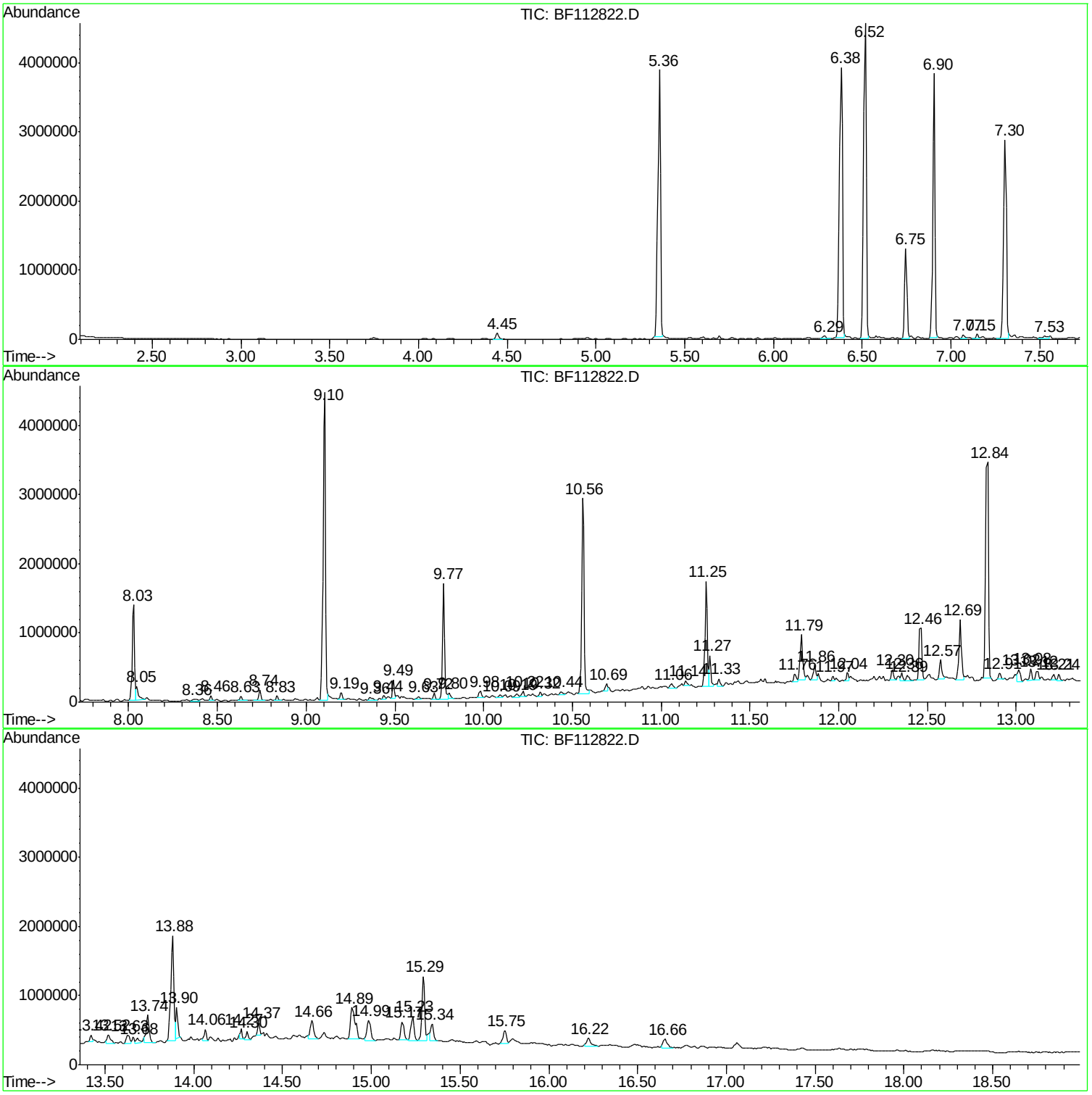
Sample : K1707-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030419\
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Operator : JU/SJ
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

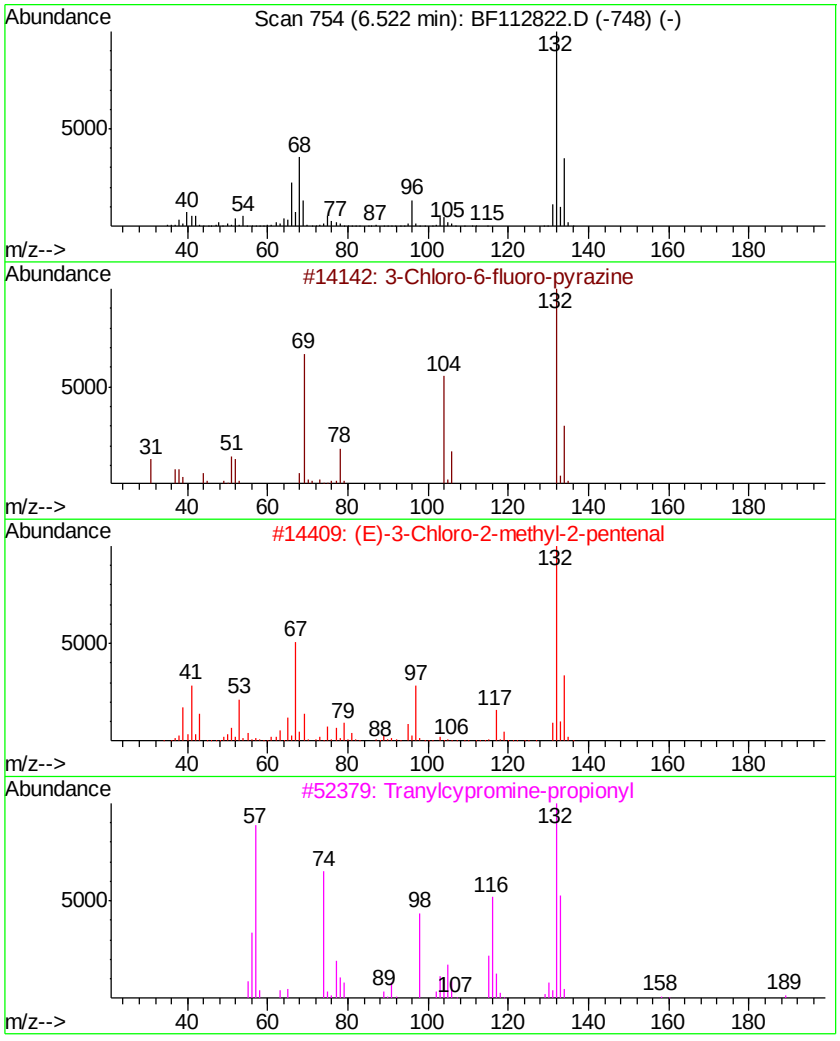
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

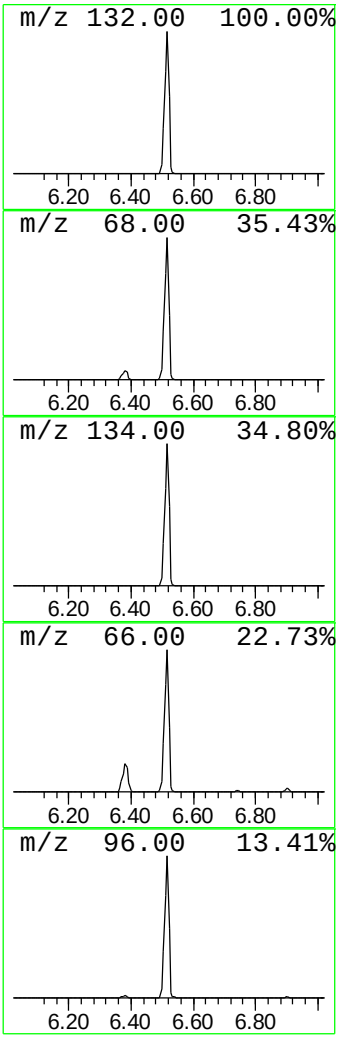
****

Peak Number 1 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	83.31 ng	4314970	1,4-Dichlorobenzene-d4	6.75

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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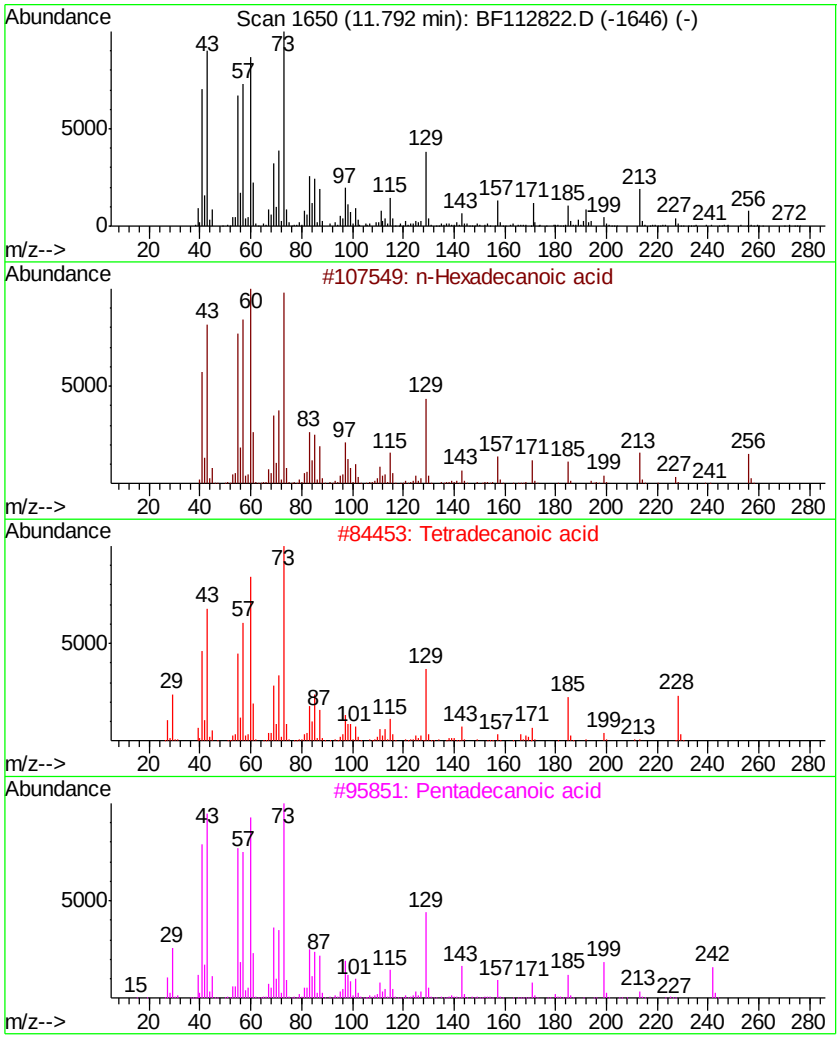
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

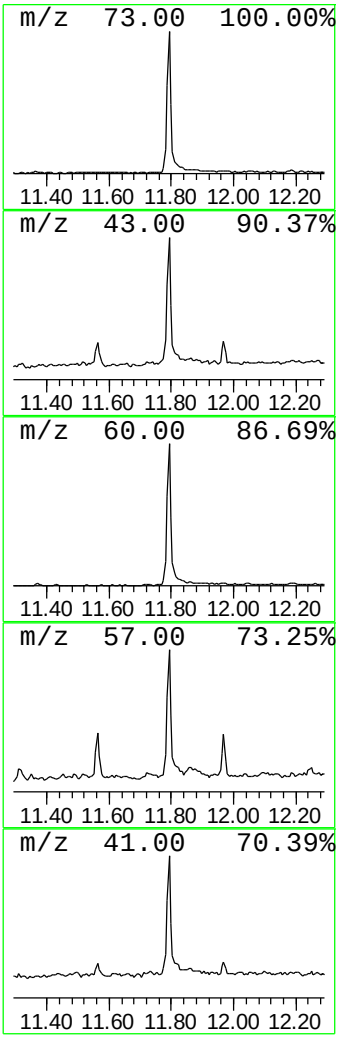
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	9.74 ng	686289	Phenanthrene-d10	11.25

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	92
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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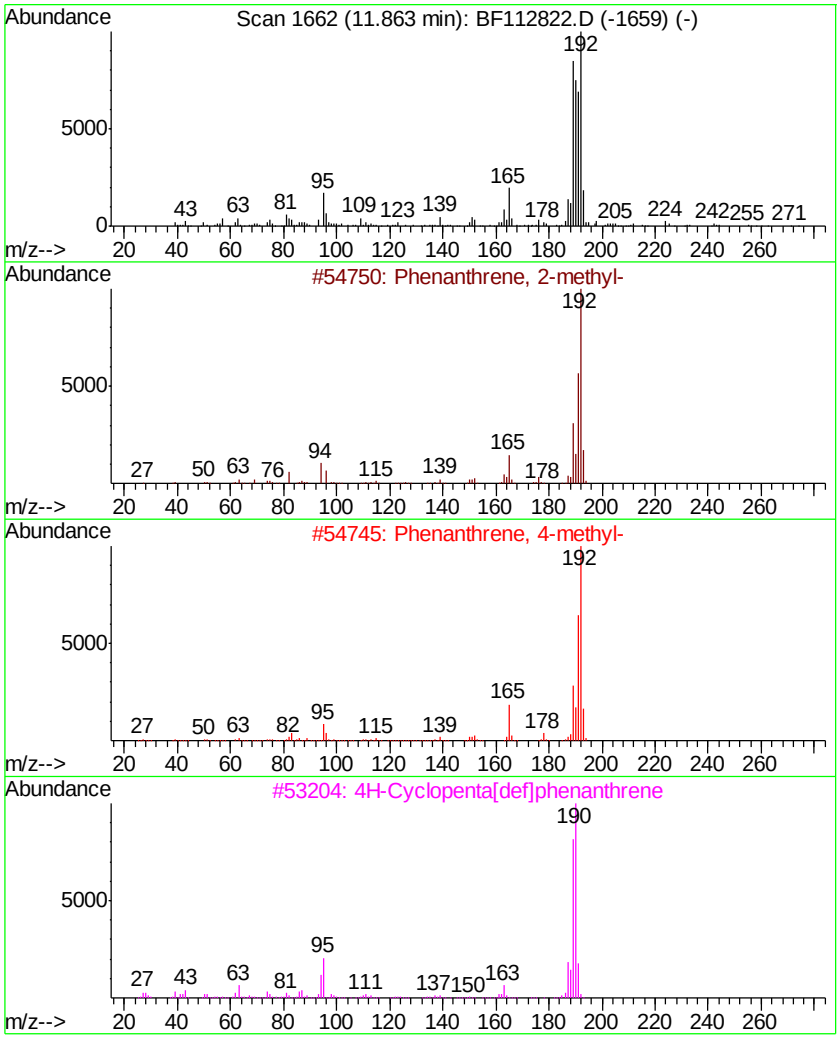
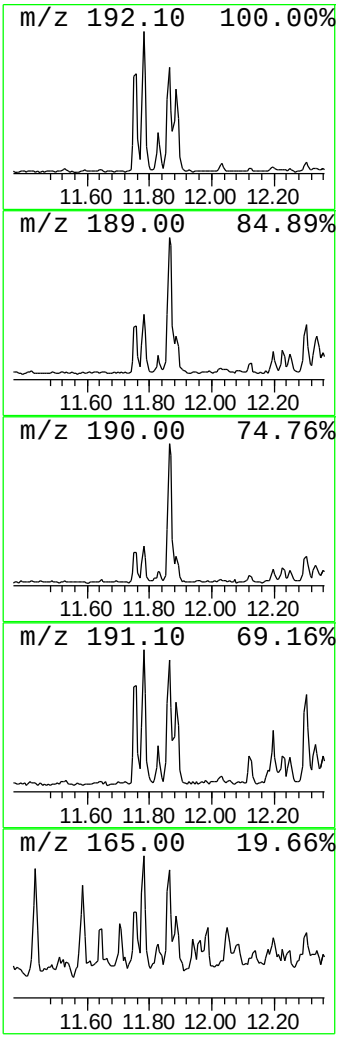
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	3.24 ng	227983	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	83
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	52
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	50





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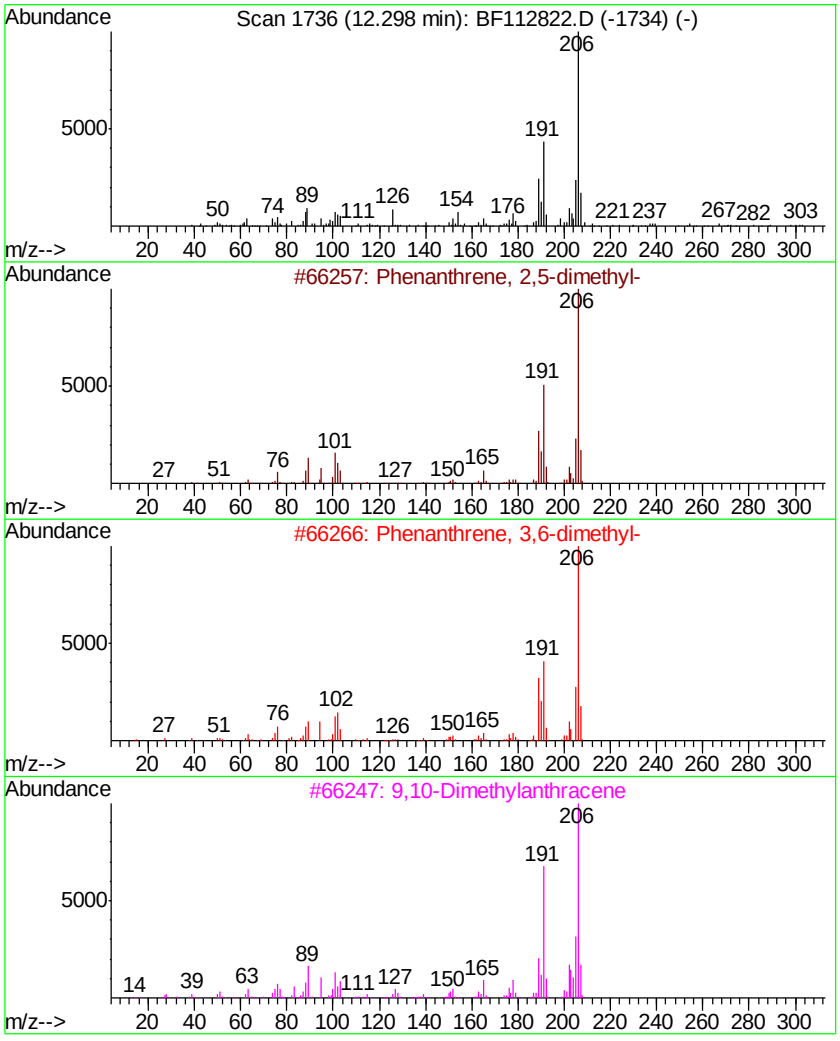
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

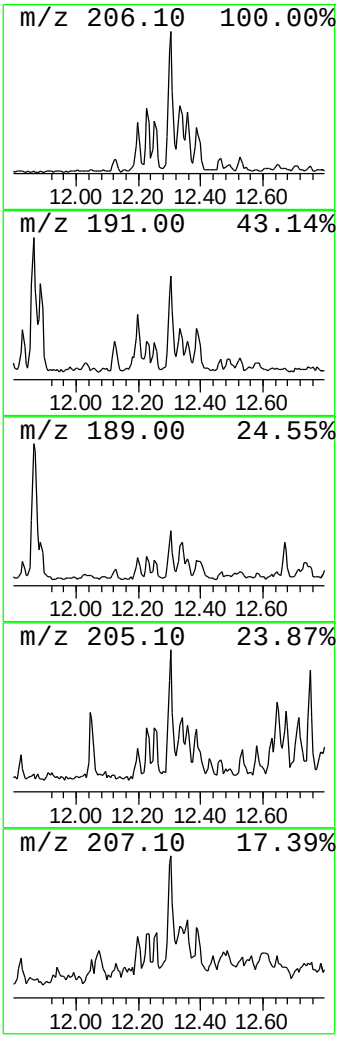
****

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.18 ng	153520	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	91
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	89
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

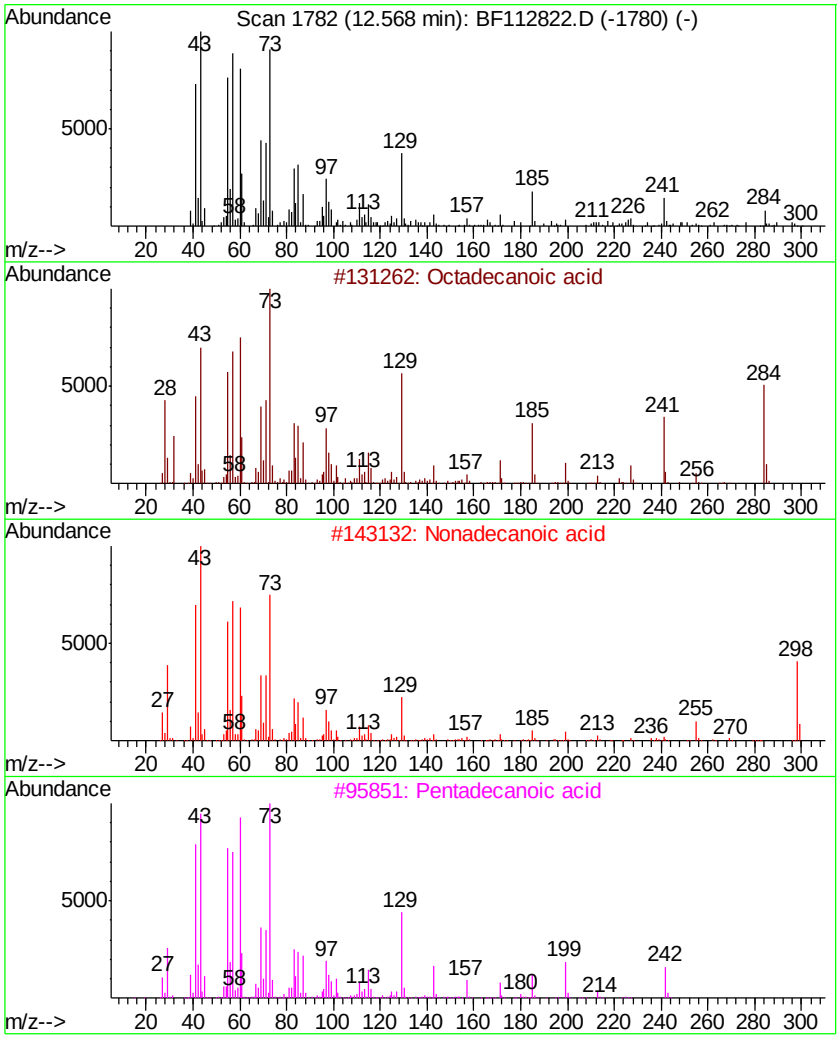
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

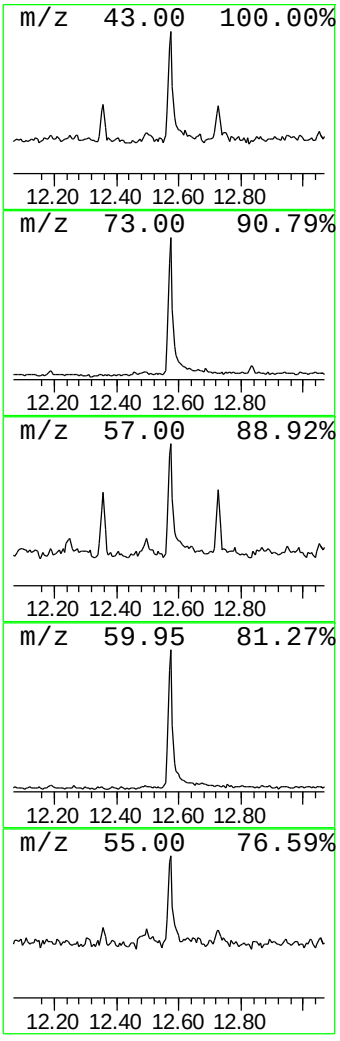
****

Peak Number 7 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.12 ng	290922	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Nonadecanoic acid	298	C19H38O2	000646-30-0	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





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Misc :
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Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

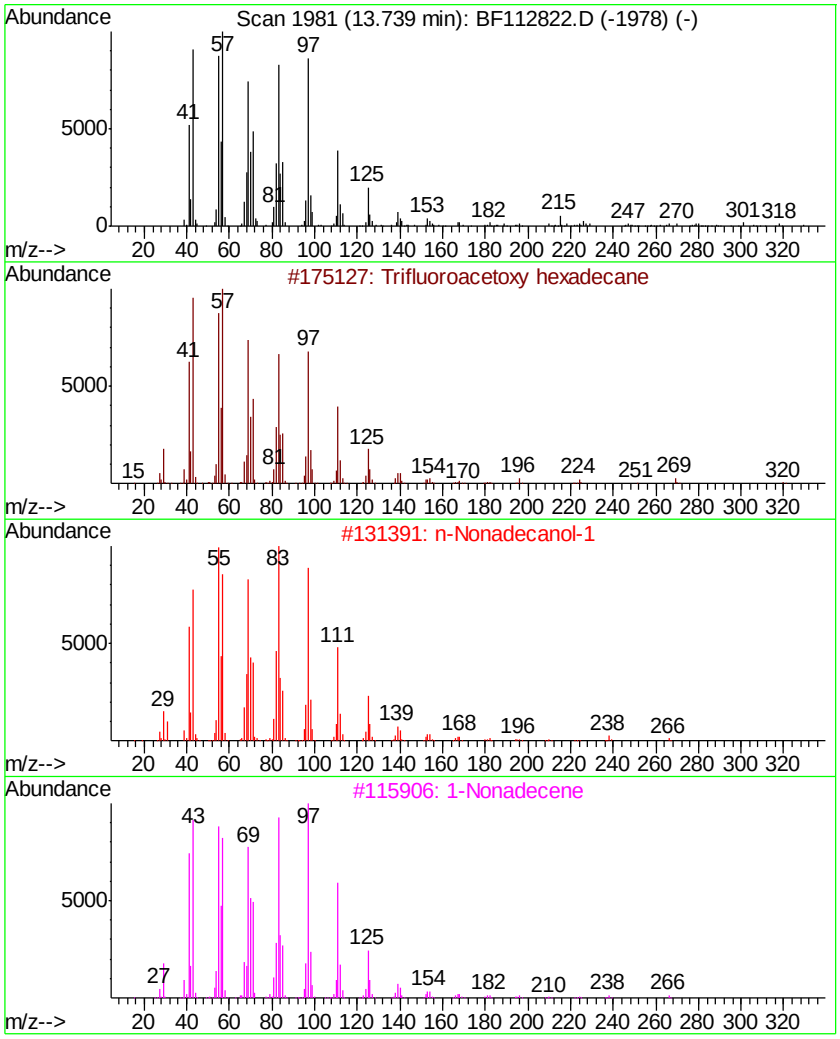
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

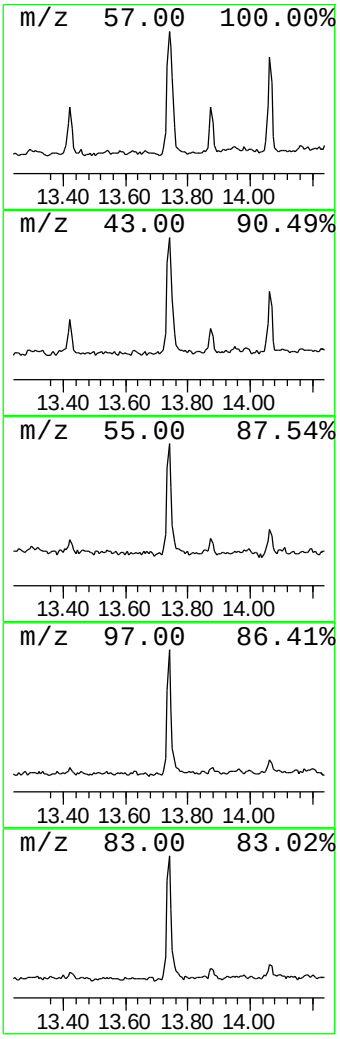
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	5.16 ng	480821	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	1-Nonadecene	266	C19H38	018435-45-5	92
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Library Search Compound Report

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Data File : BF112822.D
Acq On : 4 Mar 2019 14:18
Operator : JU/SJ
Sample : K1707-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

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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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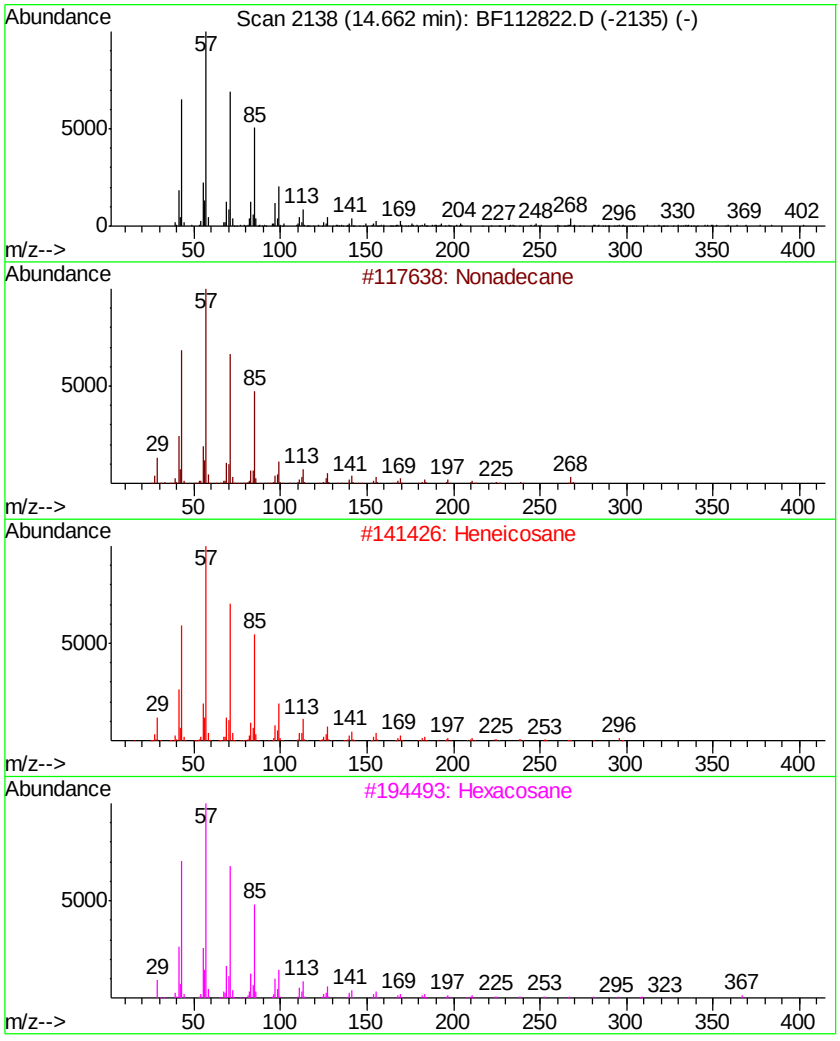
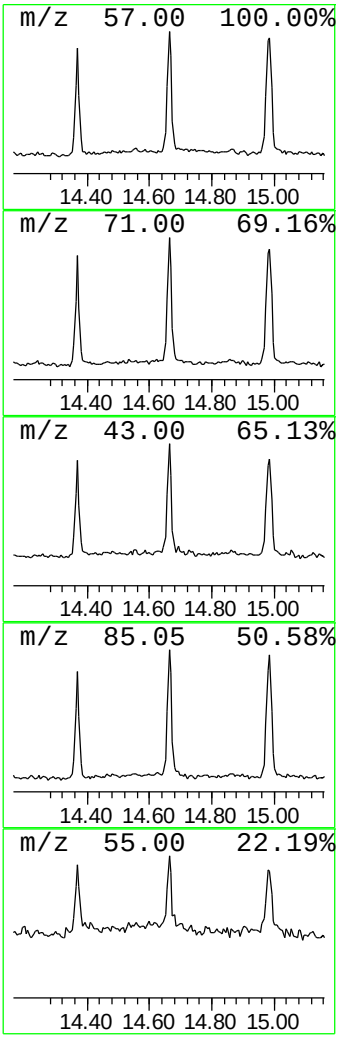
Peak Number 9 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	5.59 ng	312037	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	74
4	Eicosane	282	C20H42	000112-95-8	74
5	Tetracosane	338	C24H50	000646-31-1	72





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Misc :
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Instrument : BNA_F
ClientSampleId : S11

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

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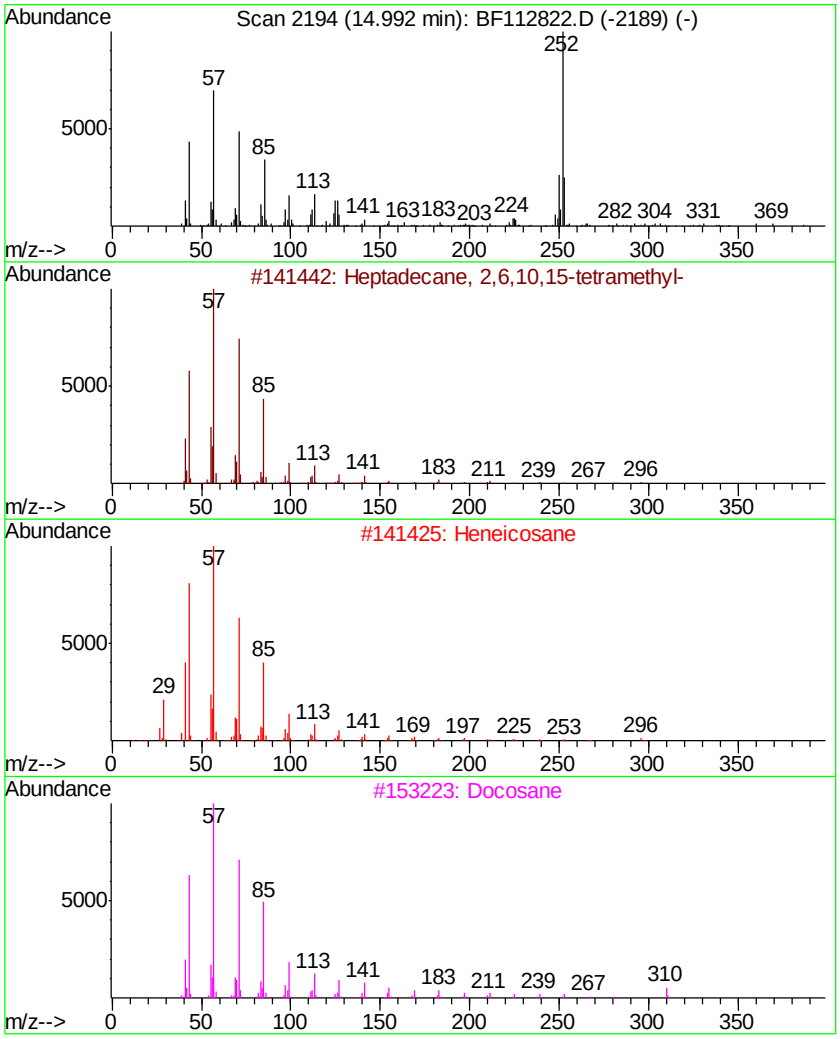
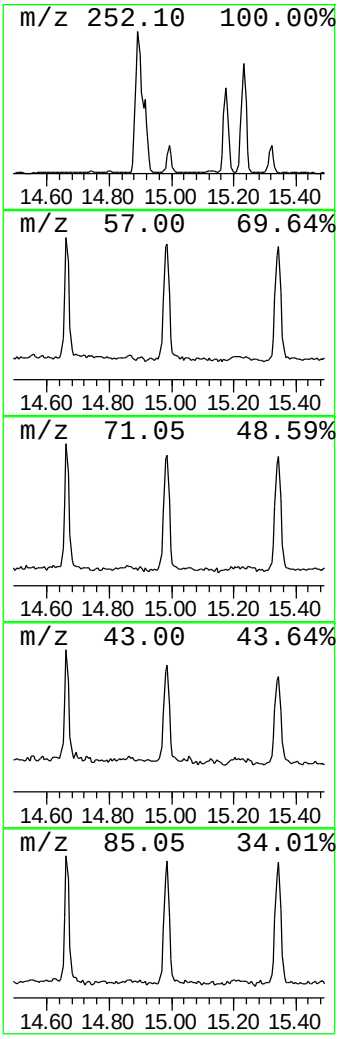
Peak Number 10 Heptadecane, 2,6,10,15-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	7.21 ng	402445	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Heneicosane	296	C21H44	000629-94-7	86
3	Docosane	310	C22H46	000629-97-0	78
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	60
5	Hexacosane	366	C26H54	000630-01-3	53





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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

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TIC Integration Parameters: LSCINT.P

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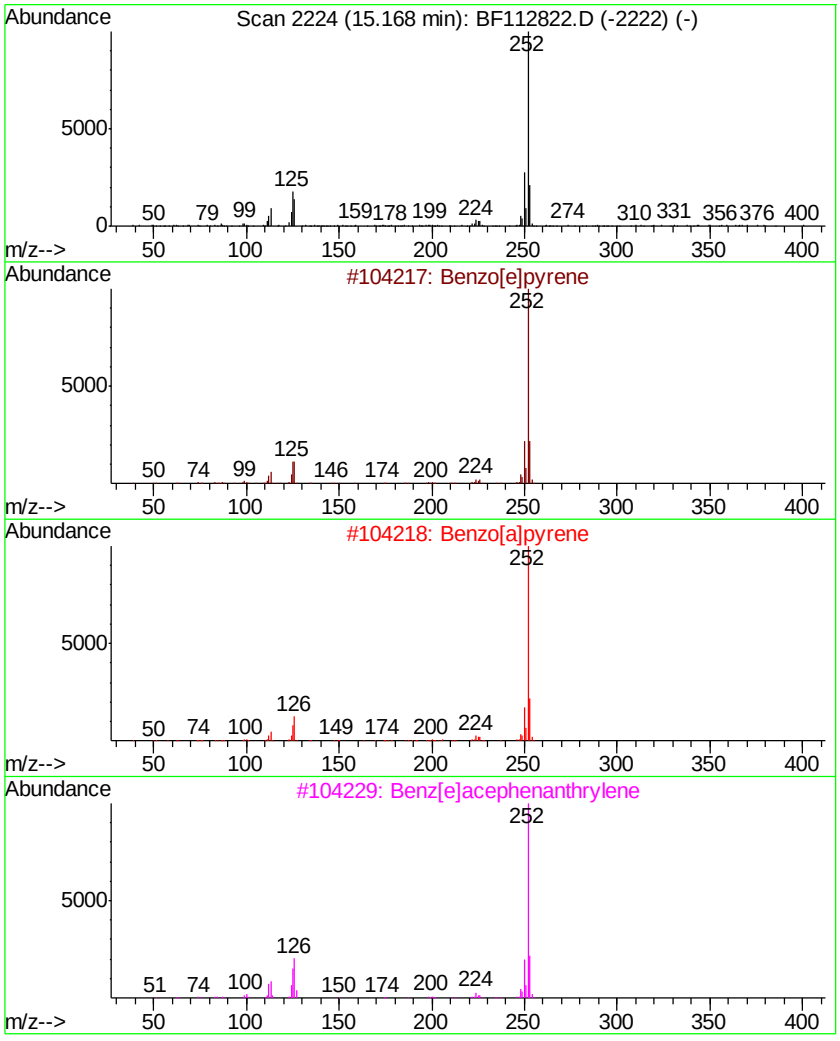
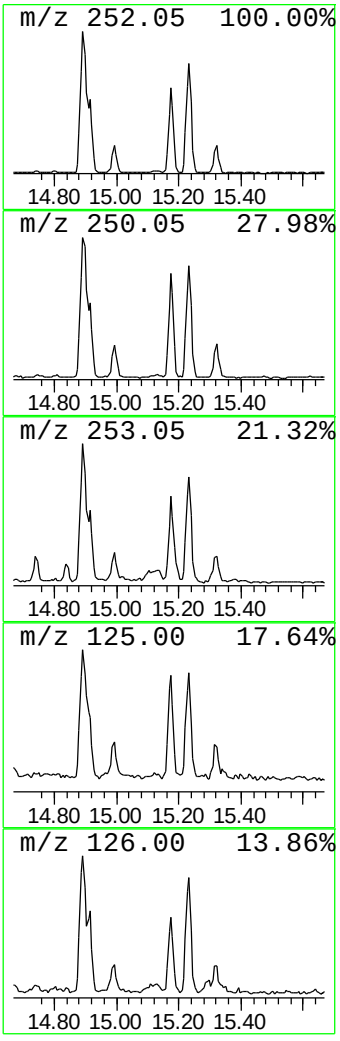
Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	5.20 ng	290084	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





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Operator : JU/SJ
Sample : K1707-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

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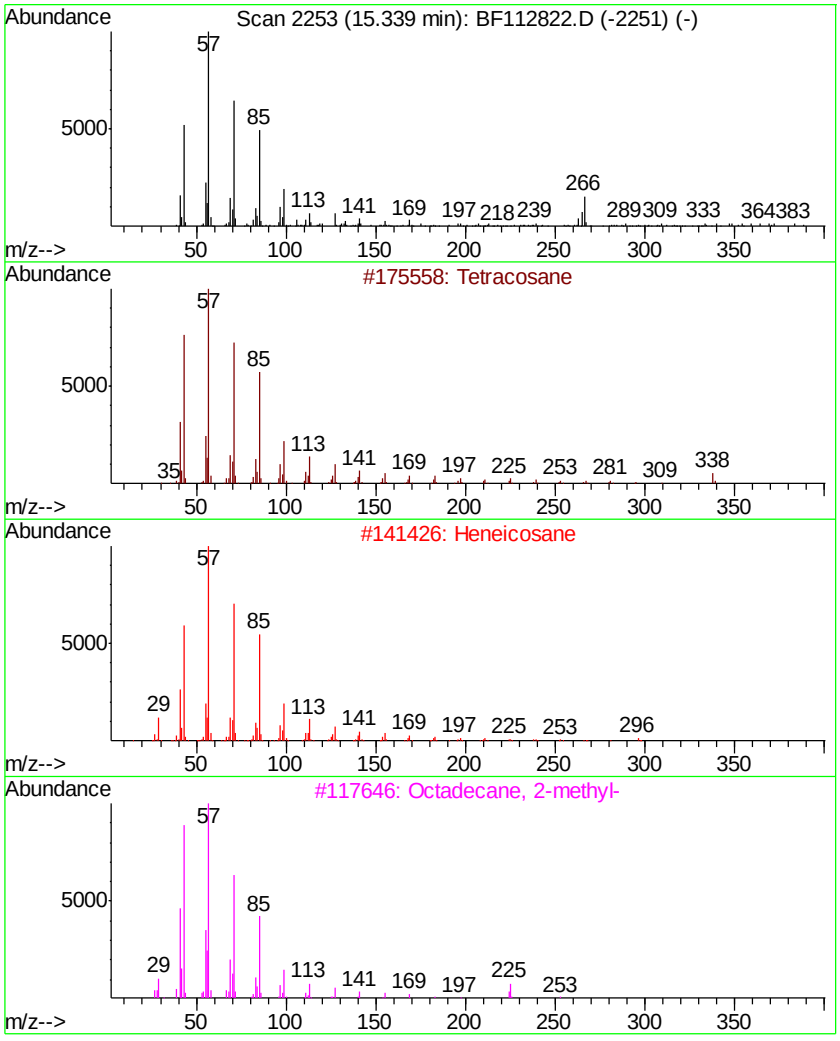
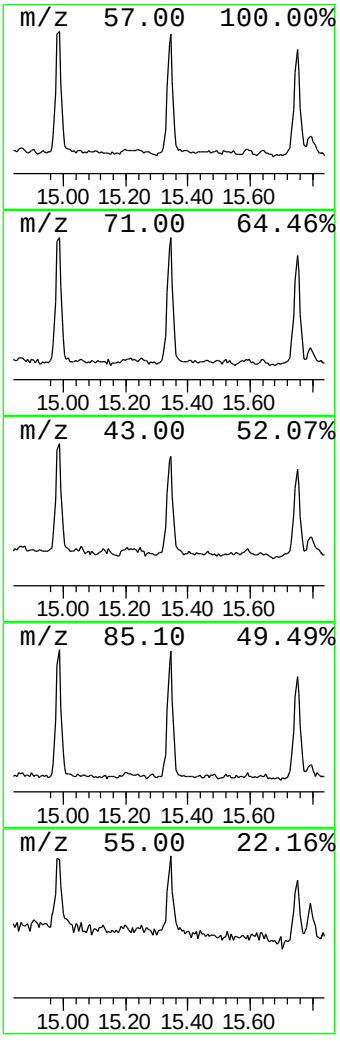
Peak Number 12 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	5.22 ng	291382	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
4	2-methyloctacosane	408	C29H60	1000376-72-8	80
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	76





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Acq On : 4 Mar 2019 14:18
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Sample : K1707-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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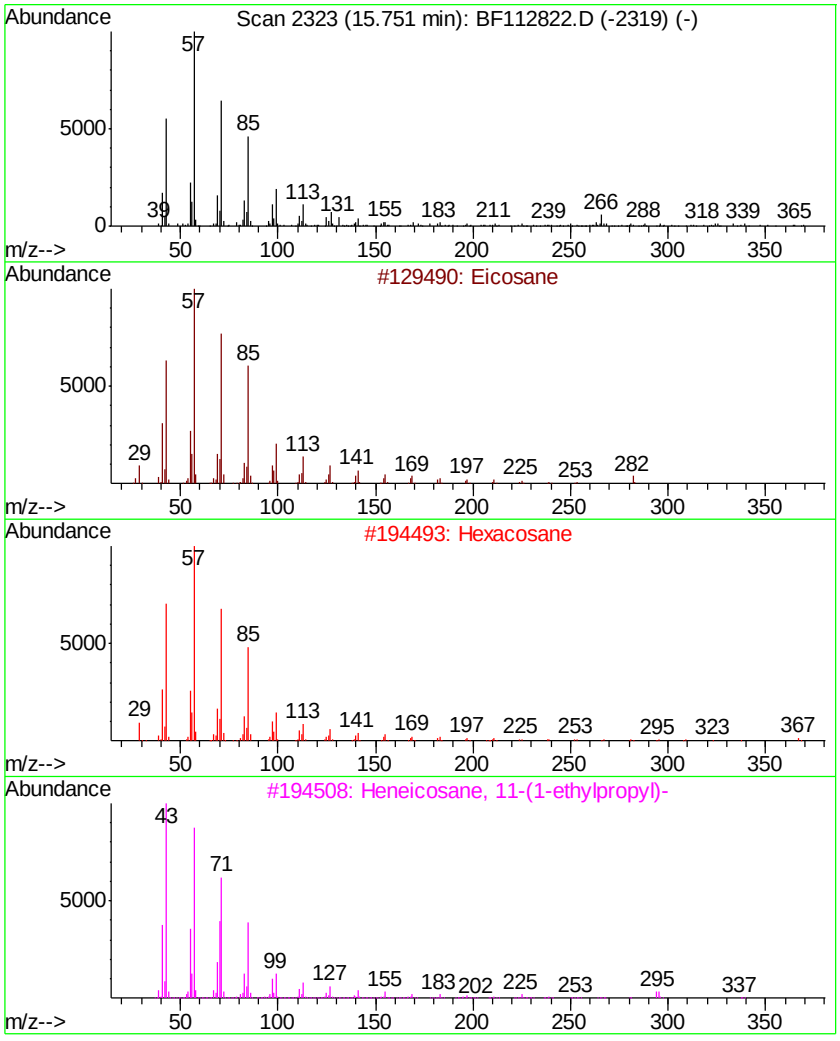
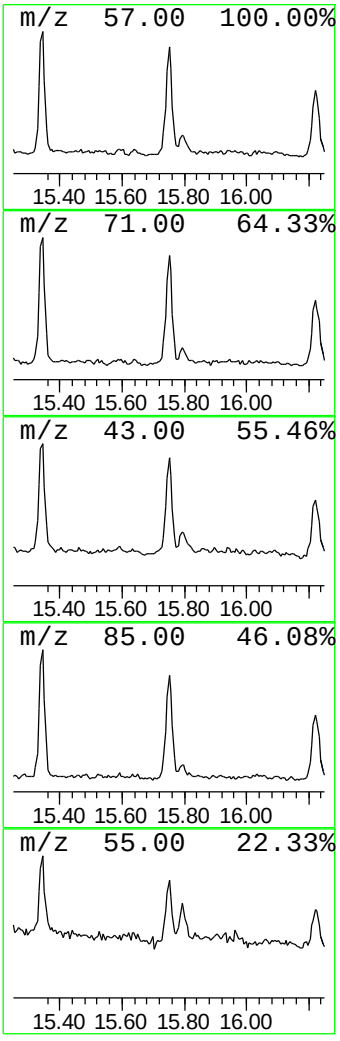
Peak Number 13 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	4.90 ng	273374	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Pentacosane	352	C25H52	000629-99-2	87





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Instrument : BNA_F
ClientSampleId : S11

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

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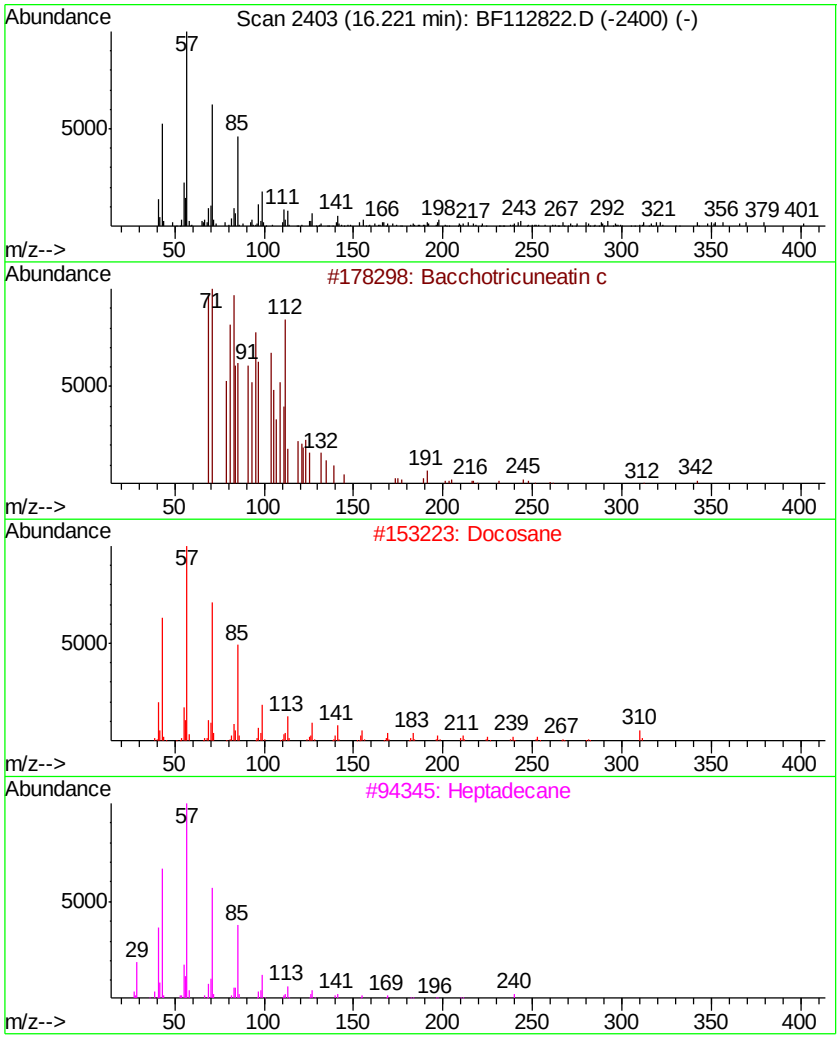
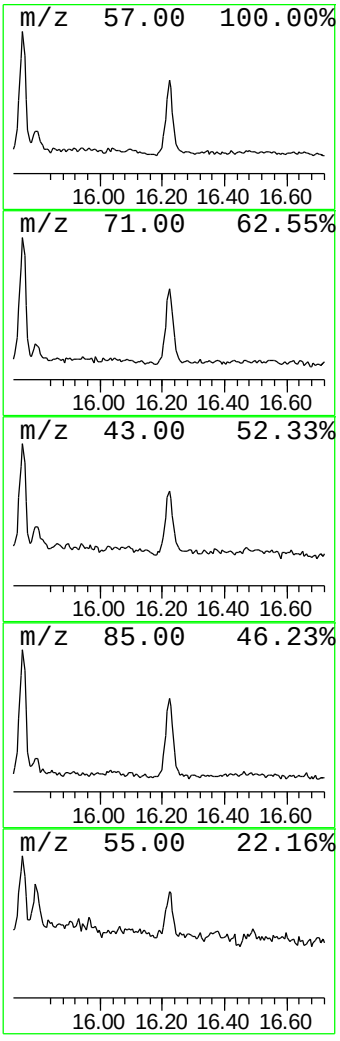
Peak Number 14 Bacchotricuneatin c Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	3.17 ng	177140	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	99
2	Docosane	310	C22H46	000629-97-0	92
3	Heptadecane	240	C17H36	000629-78-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetradecane	198	C14H30	000629-59-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030419\
Data File : BF112822.D
Acq On : 4 Mar 2019 14:18
Operator : JU/SJ
Sample : K1707-03
Misc :
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Instrument : BNA_F
ClientSampleId : S11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.52	6.52	83.3	ng	4314970	1	6.75	1035910	20.0
n-Hexadecanoic acid	11.79	9.7	ng	686289	4	11.25	1408800	20.0
Phenanthrene, 2-m...	11.86	3.2	ng	227983	4	11.25	1408800	20.0
Phenanthrene, 2,5...	12.30	2.2	ng	153520	4	11.25	1408800	20.0
Octadecanoic acid	12.57	3.1	ng	290922	5	13.88	1865110	20.0
Trifluoroacetoxy ...	13.74	5.2	ng	480821	5	13.88	1865110	20.0
Nonadecane	14.66	5.6	ng	312037	6	15.29	1115980	20.0
Heptadecane, 2,6,...	14.99	7.2	ng	402445	6	15.29	1115980	20.0
Benzo[e]pyrene	15.17	5.2	ng	290084	6	15.29	1115980	20.0
Tetracosane	15.34	5.2	ng	291382	6	15.29	1115980	20.0
Eicosane	15.75	4.9	ng	273374	6	15.29	1115980	20.0
Bacchotricuneatin c	16.22	3.2	ng	177140	6	15.29	1115980	20.0