LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103769.D
Acq On : 19 Mar 2018 21:25
Operator : JU/SJ
Sample : J1972-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-4 COMP

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-BF031518.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	2.116	3	5	14	rVB2	103646	172833	3.80%	0.405%
2	2.334	35	42	51	rVB	149257	207239	4.56%	0.486%
3	5.228	530	534	546	rVB	173246	252689	5.56%	0.592%
4	5.604	592	598	601	rBV	3961767	4415307	97.16%	10.346%
5	5.922	648	652	657	rVB	63201	63459	1.40%	0.149%
6	6.598	761	767	771	rBV	3461815	4544189	100.00%	10.648%
7	6.745	787	792	795	rBV	4006035	4470503	98.38%	10.475%
8	6.975	827	831	834	rBV	1220155	1009485	22.21%	2.365%
9	7.134	853	858	861	rBV	3609589	3443122	75.77%	8.068%
10	7.392	899	902	903	rBV	56370	45504	1.00%	0.107%
11	7.416	903	906	911	rVB	109671	136791	3.01%	0.321%
12	7.540	921	927	930	rBV	2782003	2894589	63.70%	6.783%
13	8.045	1008	1013	1016	rBV	70997	66344	1.46%	0.155%
14	8.257	1045	1049	1052	rBV	1452211	1327350	29.21%	3.110%
15	9.063	1183	1186	1190	rBV	51479	45662	1.00%	0.107%
16	9.328	1225	1231	1234	rBV	4174892	4054581	89.23%	9.501%
17	9.669	1280	1289	1291	rBV2	61471	83409	1.84%	0.195%
18	9.716	1294	1297	1300	rVB	591952	440982	9.70%	1.033%
19	9.786	1306	1309	1310	rBV2	61274	53409	1.18%	0.125%
20	9.875	1320	1324	1328	rBV2	57422	58293	1.28%	0.137%
21	9.928	1328	1333	1336	rVV	115897	88368	1.94%	0.207%
22	10.016	1344	1348	1351	rVB	1456292	1302394	28.66%	3.052%
23	10.186	1375	1377	1380	rBV	78901	73156	1.61%	0.171%
24	10.251	1385	1388	1392	rVB2	65048	58597	1.29%	0.137%
25	10.428	1416	1418	1421	rVB	144342	117936	2.60%	0.276%
26	10.563	1437	1441	1446	rVB3	56861	61235	1.35%	0.143%
27	10.710	1462	1466	1469	rBV2	52868	57108	1.26%	0.134%
28	10.804	1478	1482	1486	rBV	2260628	2347269	51.65%	5.500%
29	10.904	1496	1499	1508	rVB2	122974	164503	3.62%	0.385%
30	11.004	1513	1516	1519	rBV3	49848	52408	1.15%	0.123%
31	11.110	1529	1534	1536	rBV3	43457	66715	1.47%	0.156%
32	11.151	1538	1541	1545	rVB4	44899	65975	1.45%	0.155%
33	11.192	1545	1548	1550	rBV	57230	49973	1.10%	0.117%
34	11.322	1564	1570	1573	rBV2	76641	94000	2.07%	0.220%

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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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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.351	1573	1575	1577	rVV	74128	51973	1.14%	0.122%
36	11.504	1597	1601	1604	rBV	1189210	1123781	24.73%	2.633%
37	11.527	1604	1605	1609	rVB	270367	188828	4.16%	0.442%
38	11.580	1609	1614	1616	rBV2	43711	49585	1.09%	0.116%
39	11.616	1616	1620	1623	rVB2	153294	143610	3.16%	0.337%
40	11.957	1674	1678	1681	rBV2	50714	50753	1.12%	0.119%
41	12.016	1684	1688	1690	rBV2	234620	263260	5.79%	0.617%
42	12.116	1702	1705	1707	rBV2	89646	102017	2.24%	0.239%
43	12.139	1707	1709	1714	rVB2	99958	102214	2.25%	0.240%
44	12.192	1714	1718	1720	rBV2	47830	53915	1.19%	0.126%
45	12.333	1739	1742	1746	rVB4	40758	54511	1.20%	0.128%
46	12.557	1777	1780	1782	rBV	65709	62613	1.38%	0.147%
47	12.645	1792	1795	1799	rBV3	43375	50975	1.12%	0.119%
48	12.722	1805	1808	1812	rBV	393501	322844	7.10%	0.756%
49	12.898	1836	1838	1842	rBV5	38173	49226	1.08%	0.115%
50	12.957	1842	1848	1853	rVB	346251	412234	9.07%	0.966%
51	13.092	1867	1871	1875	rVB	2837363	2825949	62.19%	6.622%
52	13.169	1880	1884	1889	rBV3	44056	71851	1.58%	0.168%
53	13.280	1900	1903	1906	rVB2	74842	68171	1.50%	0.160%
54	13.386	1917	1921	1924	rBV2	69271	72394	1.59%	0.170%
55	13.751	1981	1983	1986	rBV	86968	74561	1.64%	0.175%
56	13.792	1987	1990	1994	rVB	48119	53865	1.19%	0.126%
57	13.933	2011	2014	2016	rVV	75497	63945	1.41%	0.150%
58	13.974	2018	2021	2030	rVB3	568245	657291	14.46%	1.540%
59	14.157	2047	2052	2055	rBV2	1070389	1237613	27.24%	2.900%
60	14.198	2055	2059	2062	rVB2	304870	396456	8.72%	0.929%
61	14.304	2074	2077	2082	rBV3	42805	57224	1.26%	0.134%
62	14.551	2117	2119	2122	rVB2	68806	57130	1.26%	0.134%
63	14.621	2128	2131	2138	rVB3	126060	154445	3.40%	0.362%
64	15.239	2232	2236	2239	rBV	146260	214811	4.73%	0.503%
65	15.321	2247	2250	2253	rVB3	67206	73256	1.61%	0.172%
66	15.563	2288	2291	2297	rVB	86756	115681	2.55%	0.271%
67	15.627	2299	2302	2307	rVB	112067	138410	3.05%	0.324%
68	15.698	2309	2314	2318	rBV2	561119	742802	16.35%	1.741%
69	16.227	2400	2404	2413	rVB6	70466	133212	2.93%	0.312%

Sum of corrected areas: 42676783

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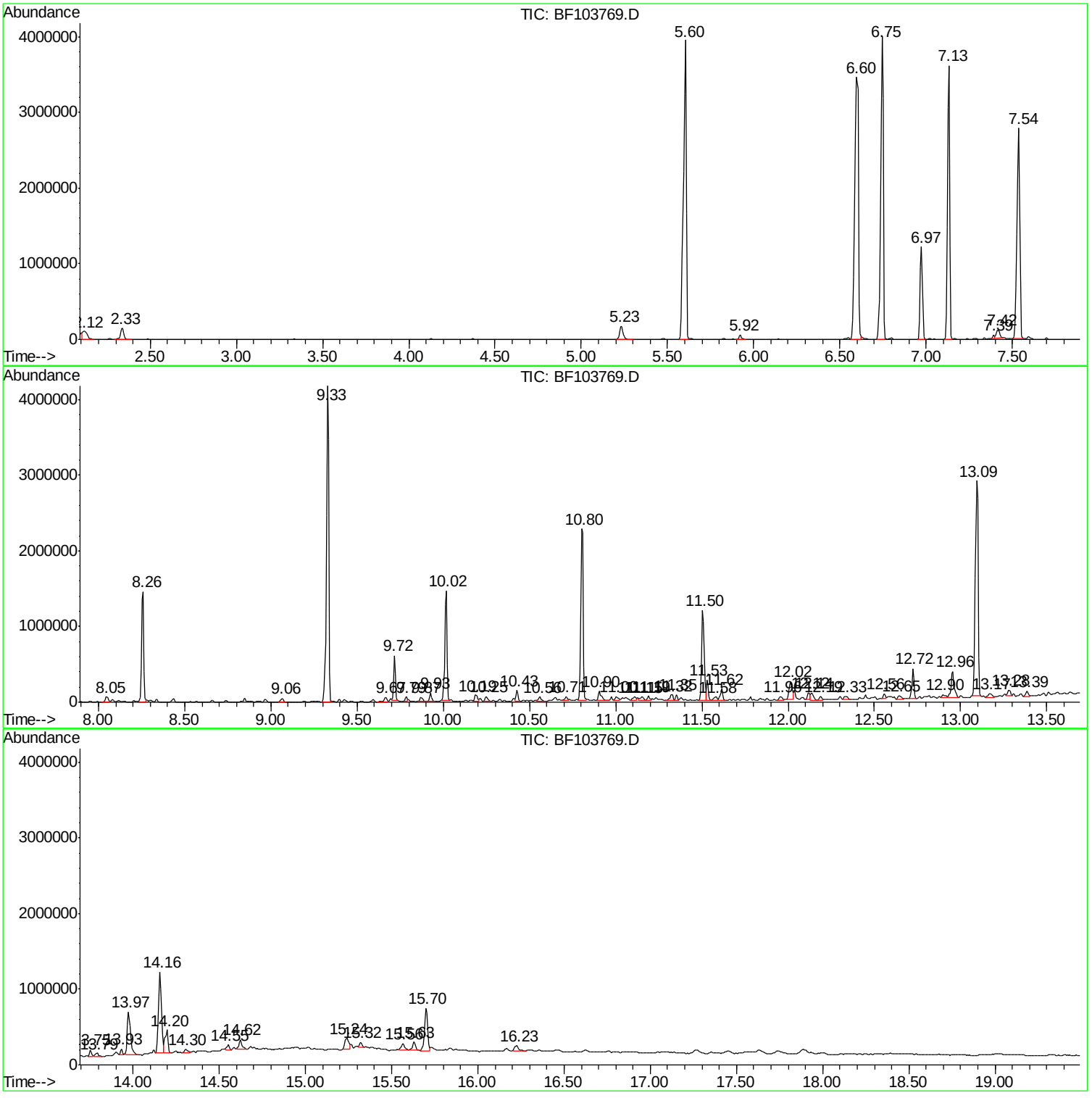
Instrument : BNA_F
ClientSampleId : S-4 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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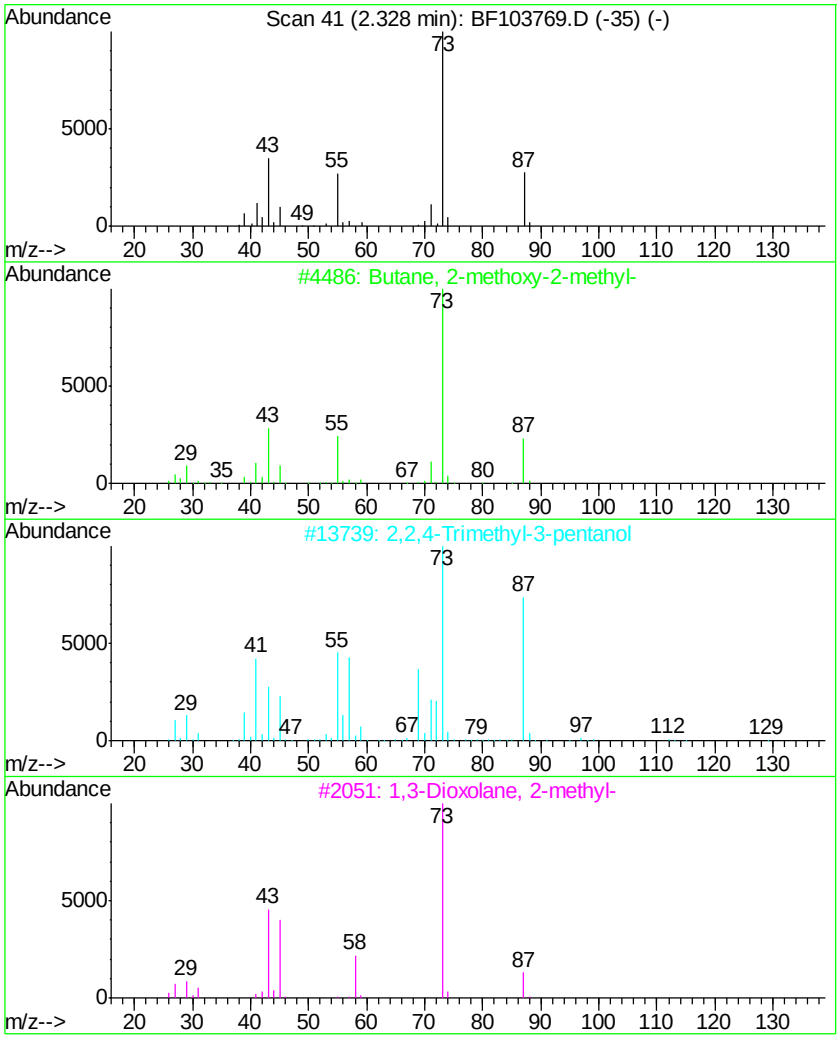
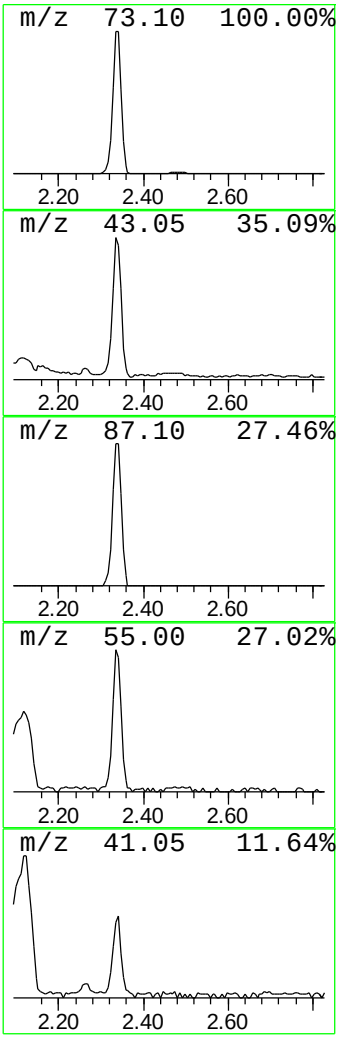
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	4.11 ng	207239	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23





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Operator : JU/SJ
Sample : J1972-08
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ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-4 COMP

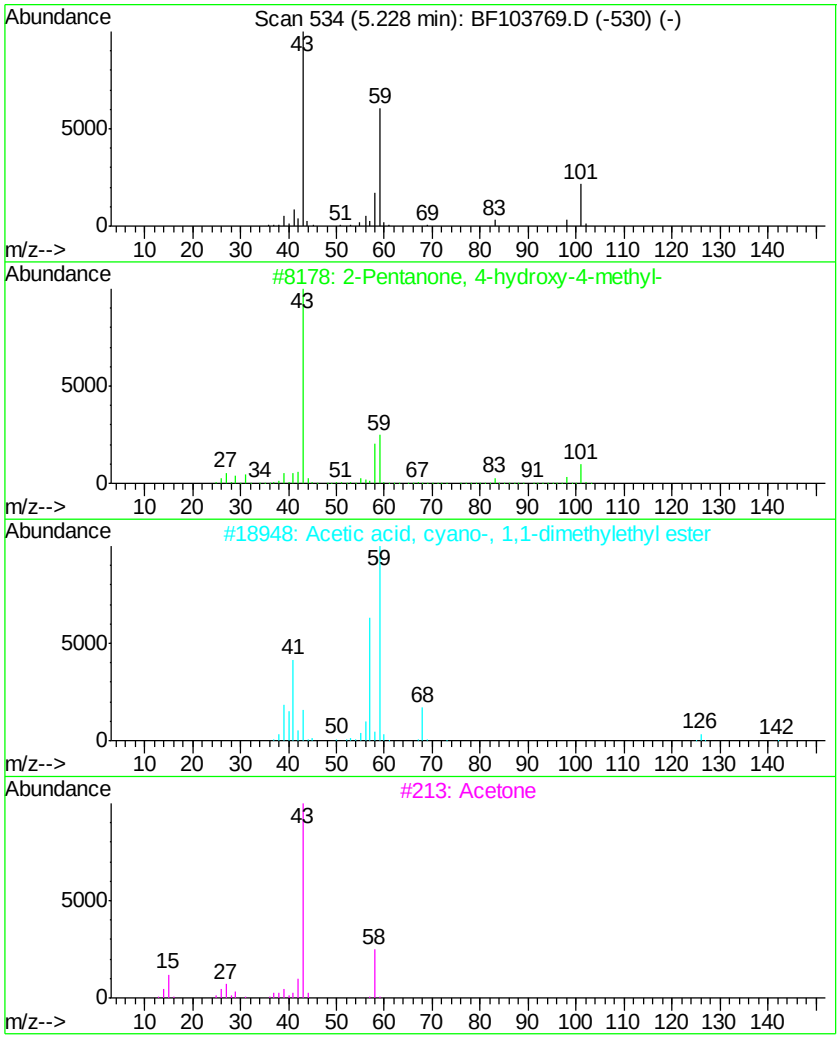
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

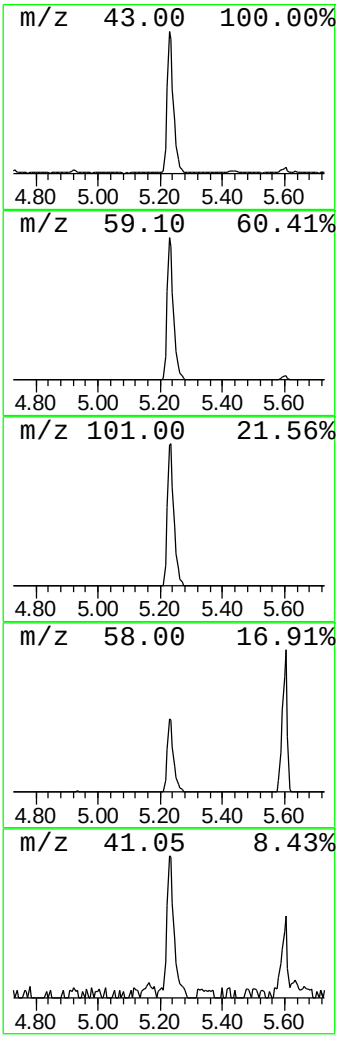
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	5.01 ng	252689	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Acetone	58	C3H6O	000067-64-1	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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TIC Library : C:\DATABASE\NIST11.L
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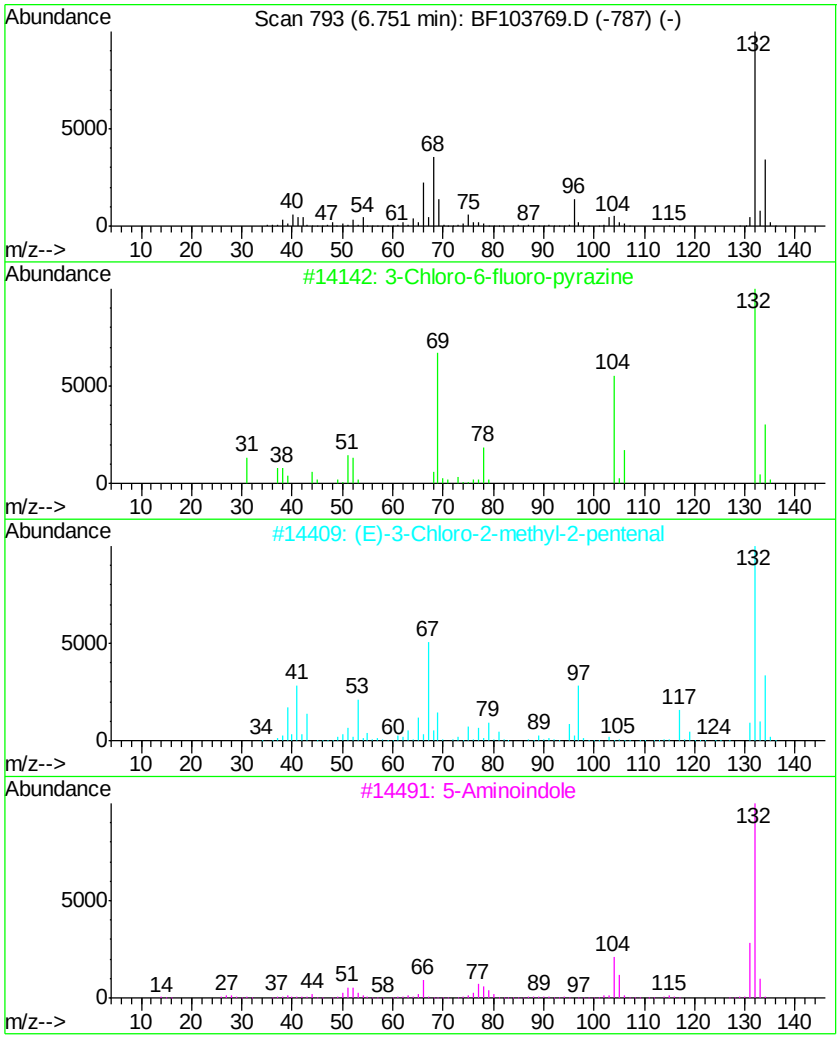
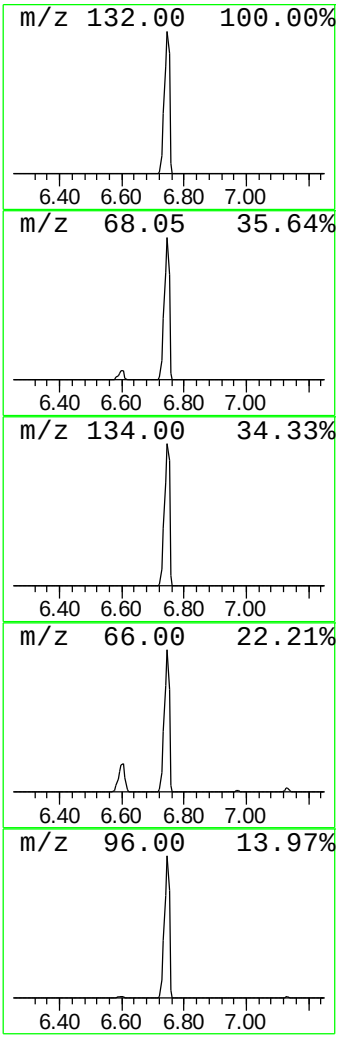
Peak Number 4 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	88.57 ng	4470500	1,4-Dichlorobenzene-d4	6.97

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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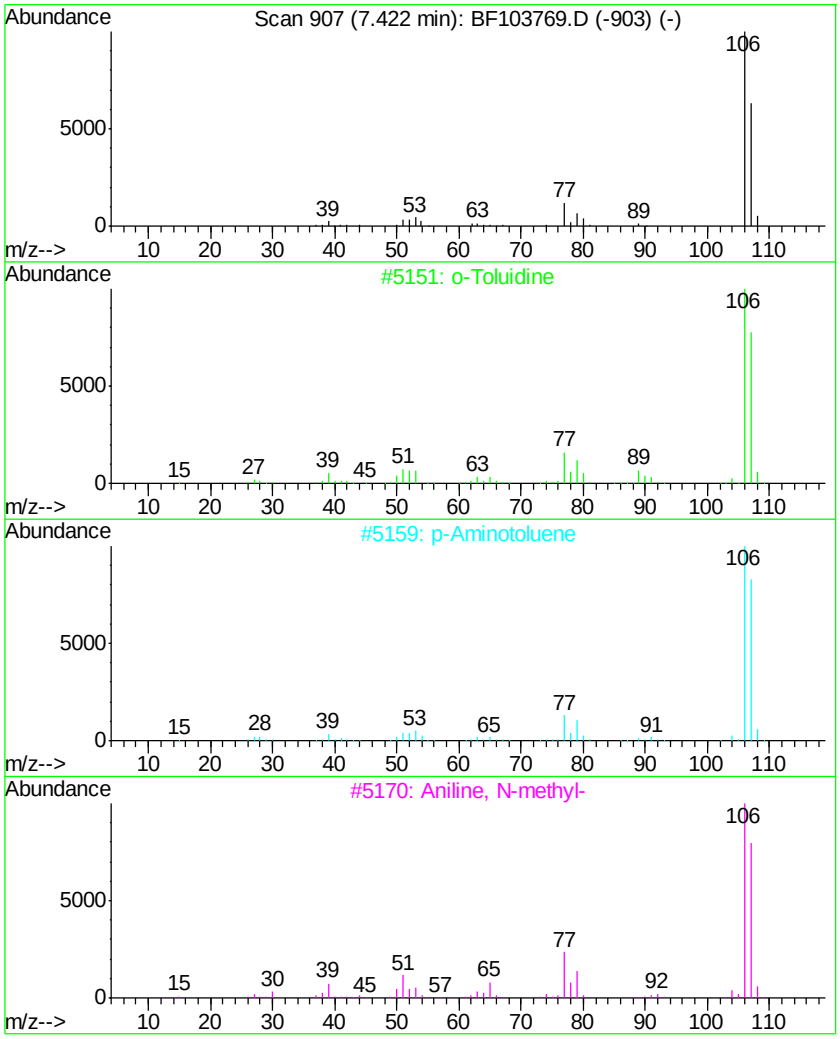
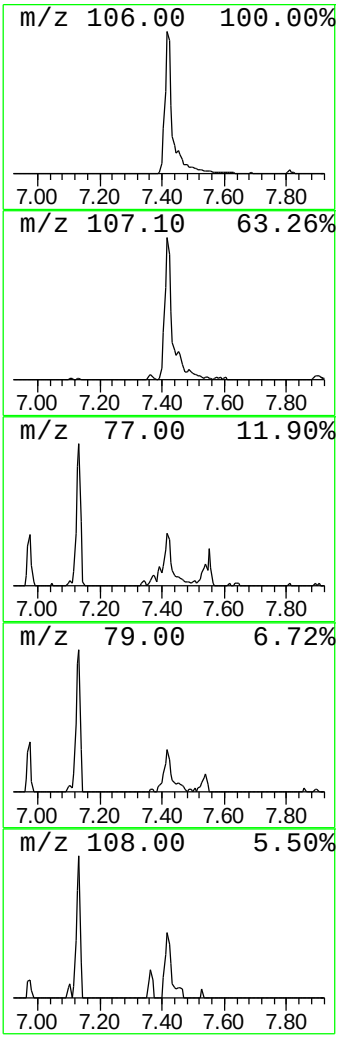
Peak Number 6 o-Toluidine Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	2.71 ng	136791	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Toluidine	107	C7H9N	000095-53-4	91
2	p-Aminotoluene	107	C7H9N	000106-49-0	90
3	Aniline, N-methyl-	107	C7H9N	000100-61-8	78
4	Pyridine, 2,5-dimethyl-	107	C7H9N	000589-93-5	78
5	Pyridine, 2-ethyl-	107	C7H9N	000100-71-0	72





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TIC Library : C:\DATABASE\NIST11.L
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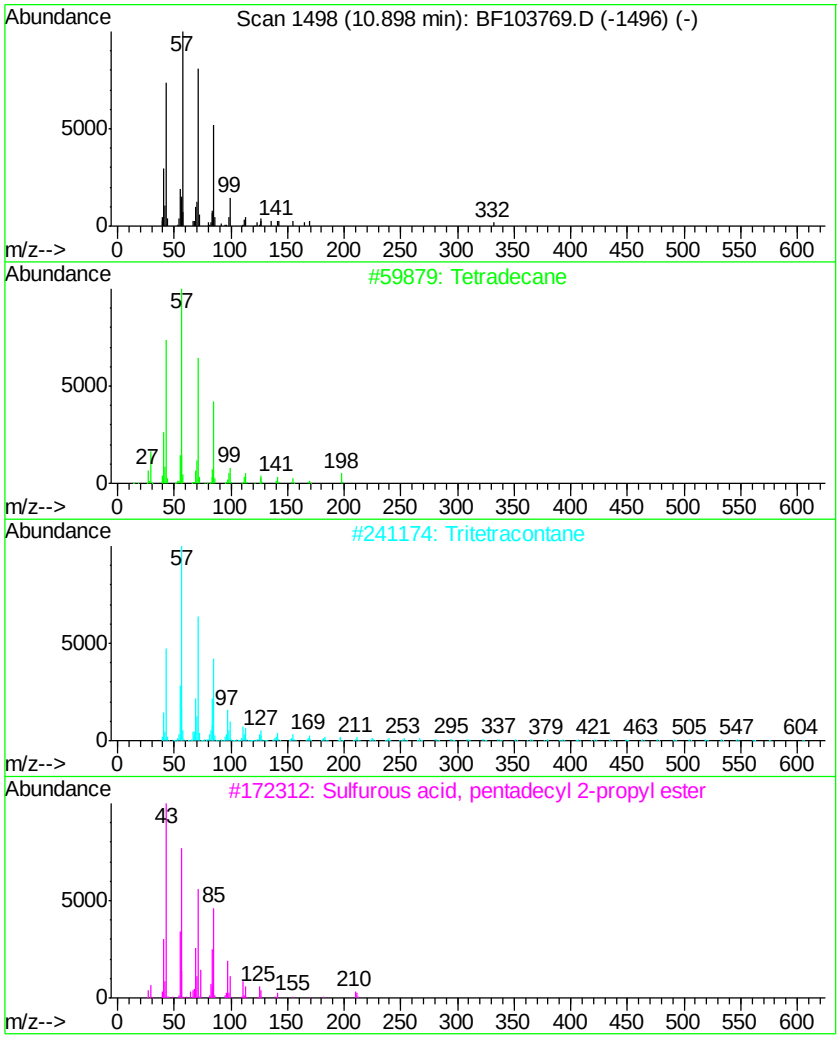
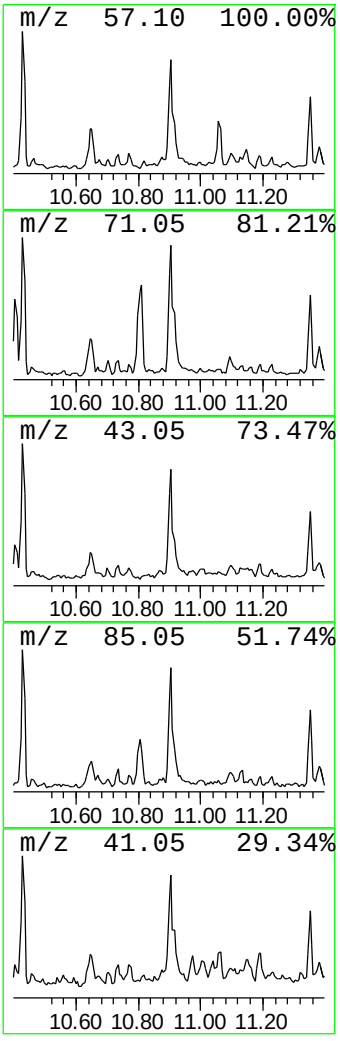
Peak Number 7 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.93 ng	164503	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Tritetracontane	605	C43H88	007098-21-7	90
3	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentadecane	212	C15H32	000629-62-9	87





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

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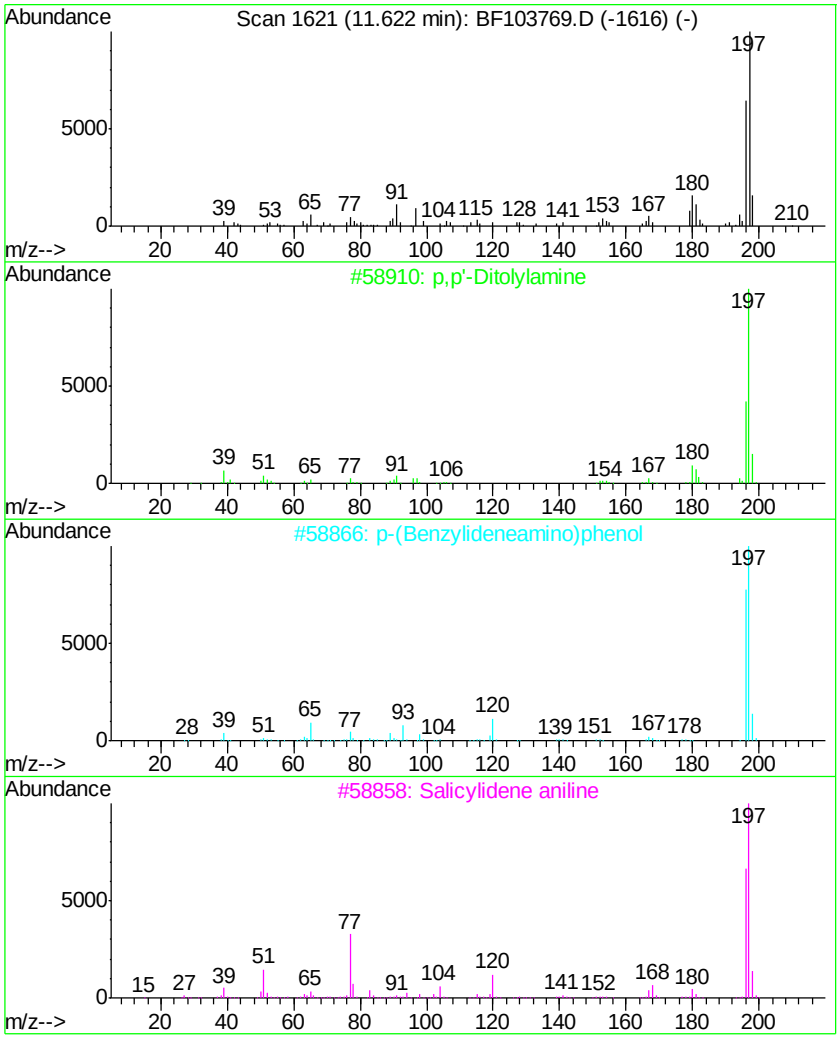
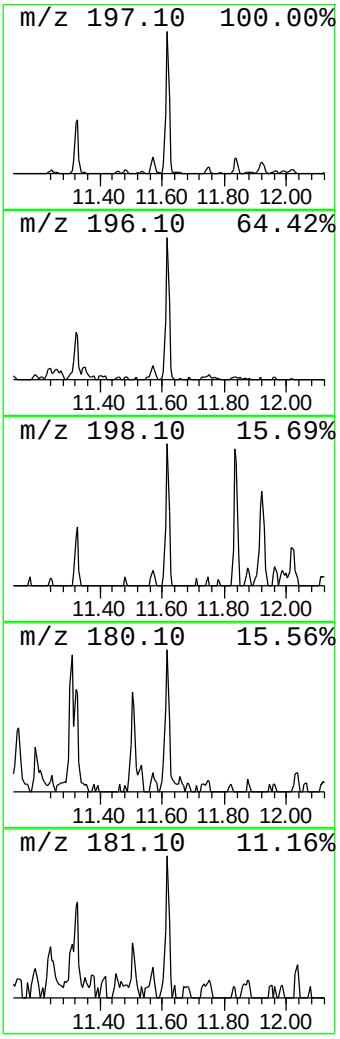
Peak Number 8 p,p'-Ditolylamine Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	2.56 ng	143610	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p,p'-Ditolylamine	197	C14H15N	000620-93-9	86
2	p-(Benzylideneamino)phenol	197	C13H11NO	000588-53-4	62
3	Salicylidene aniline	197	C13H11NO	000779-84-0	59
4	Benzo[g]quinolin-4(1H)-one, 2,3-...	197	C13H11NO	021516-07-4	59
5	1-Hydroxy-3-methyl-9H-carbazol	197	C13H11NO	014960-81-7	59





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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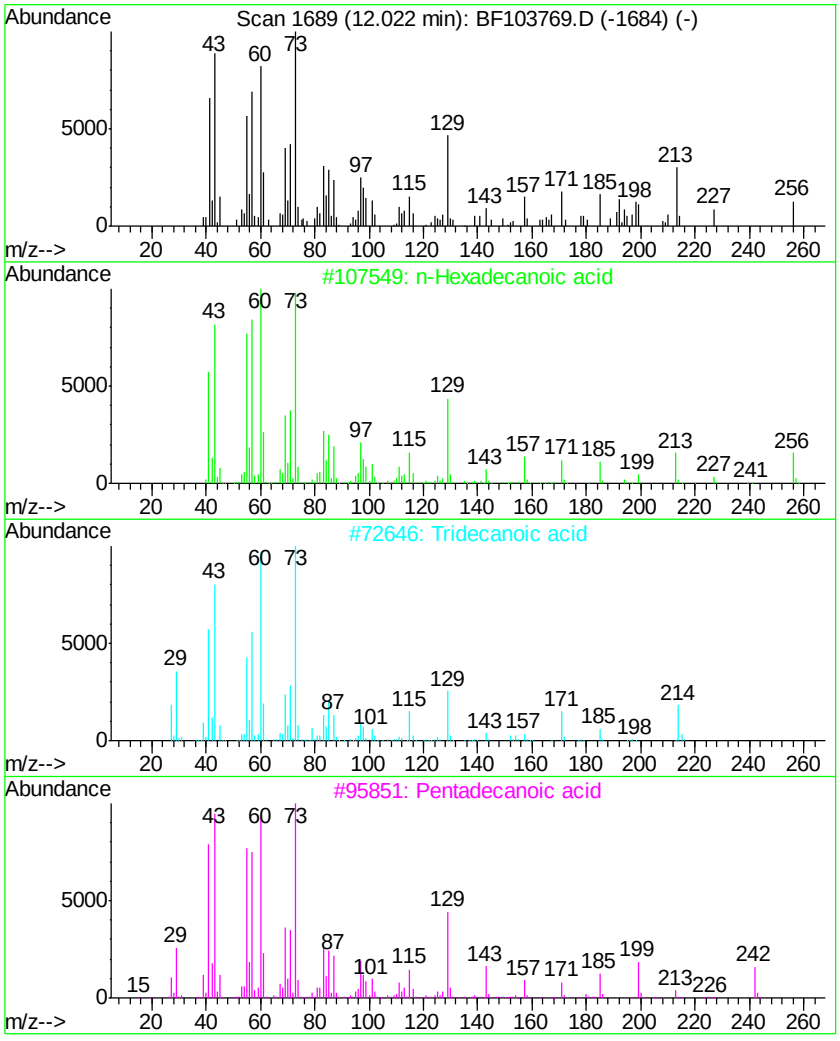
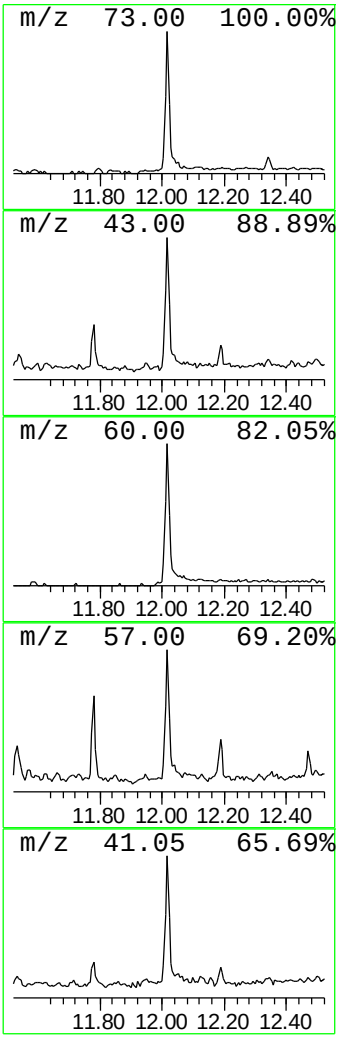
Peak Number 9 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	4.69 ng	263260	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





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Data File : BF103769.D
Acq On : 19 Mar 2018 21:25
Operator : JU/SJ
Sample : J1972-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-4 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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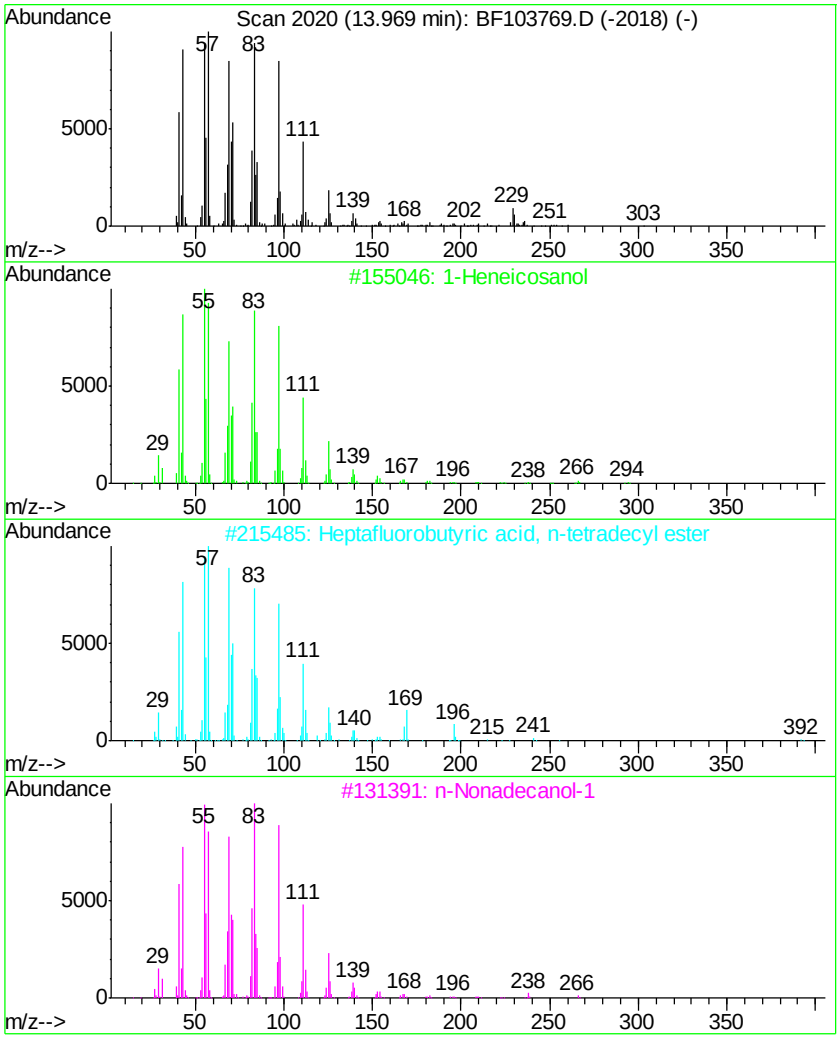
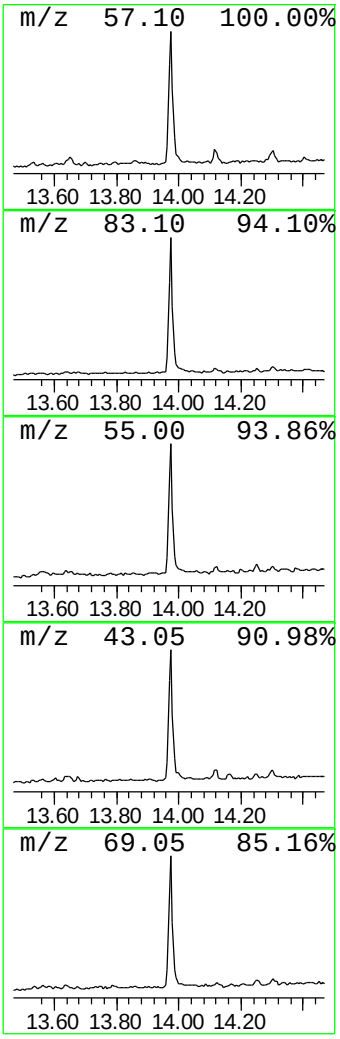
Peak Number 10 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	10.62 ng	657291	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





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Instrument : BNA_F
ClientSampleId : S-4 COMP

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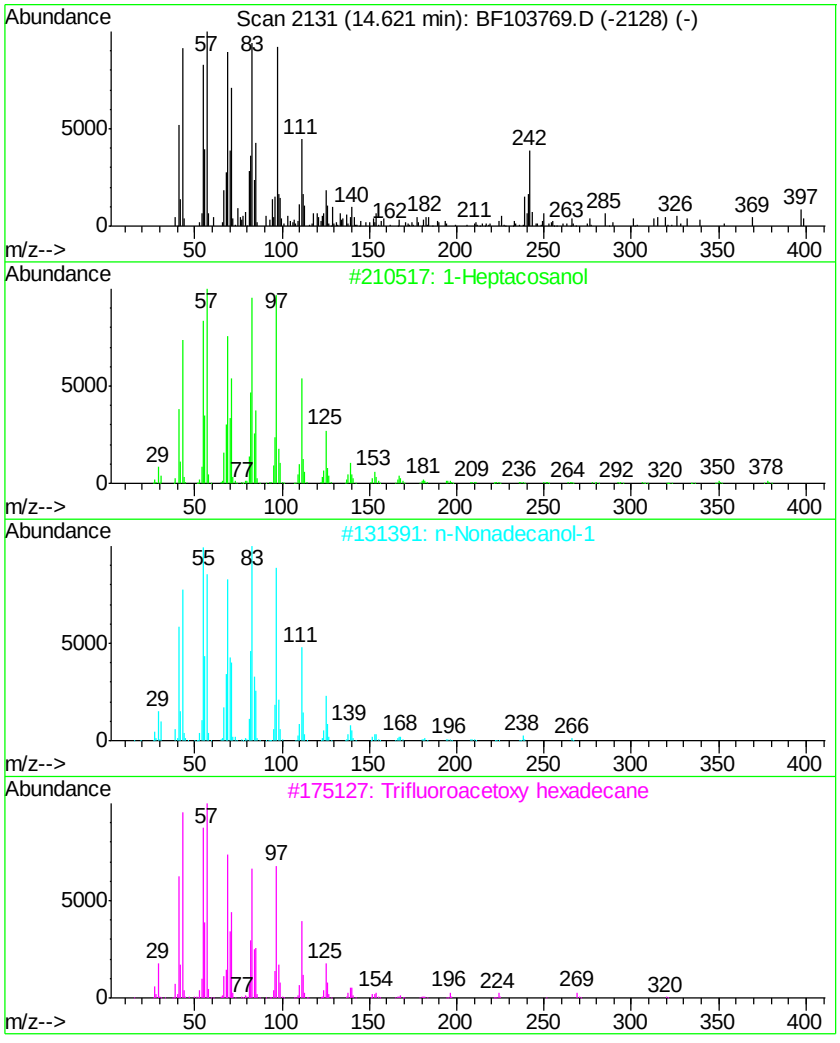
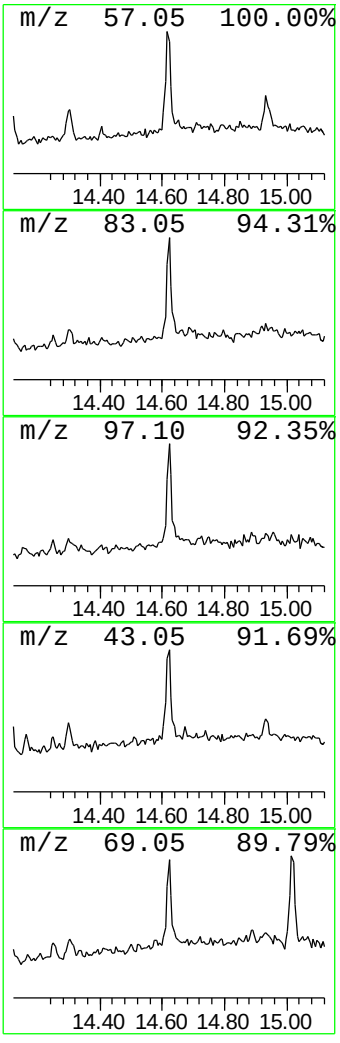
Peak Number 11 1-Heptacosanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.50 ng	154445	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	87
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	81
4	1-Heneicosanol	312	C21H44O	015594-90-8	81
5	Behenic alcohol	326	C22H46O	000661-19-8	81





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103769.D
Acq On : 19 Mar 2018 21:25
Operator : JU/SJ
Sample : J1972-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-4 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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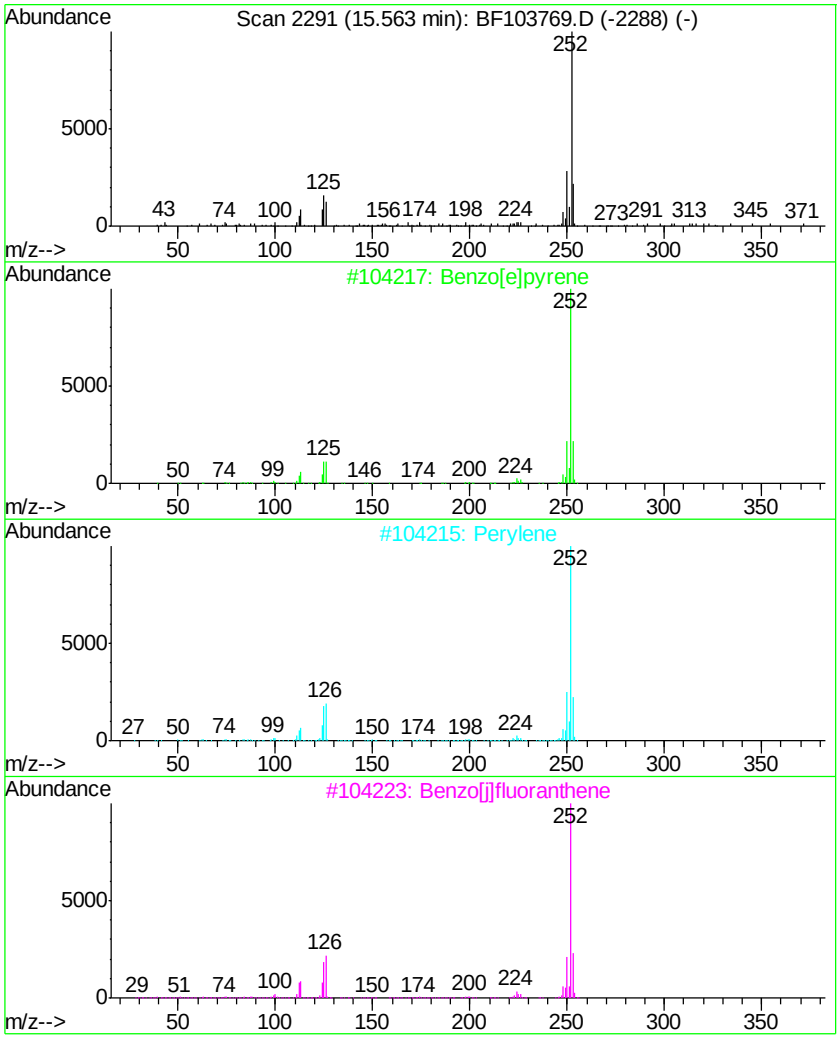
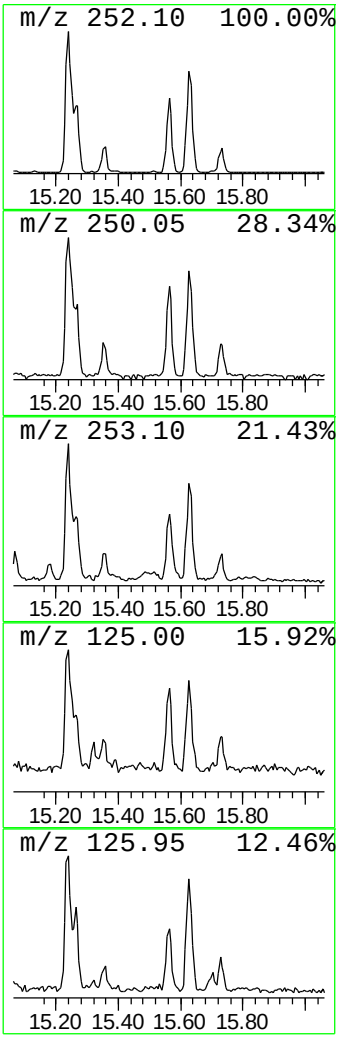
Peak Number 12 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	3.11 ng	115681	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Perylene	252	C20H12	000198-55-0	89
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	89
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





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Operator : JU/SJ
Sample : J1972-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-4 COMP

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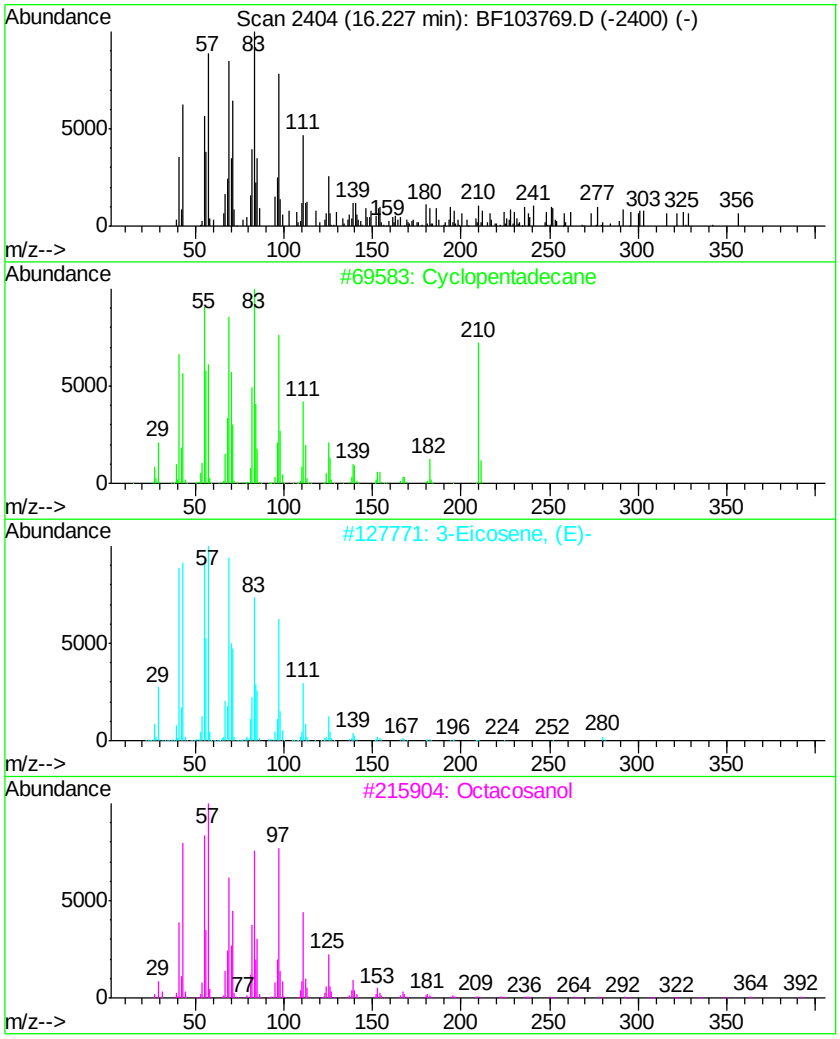
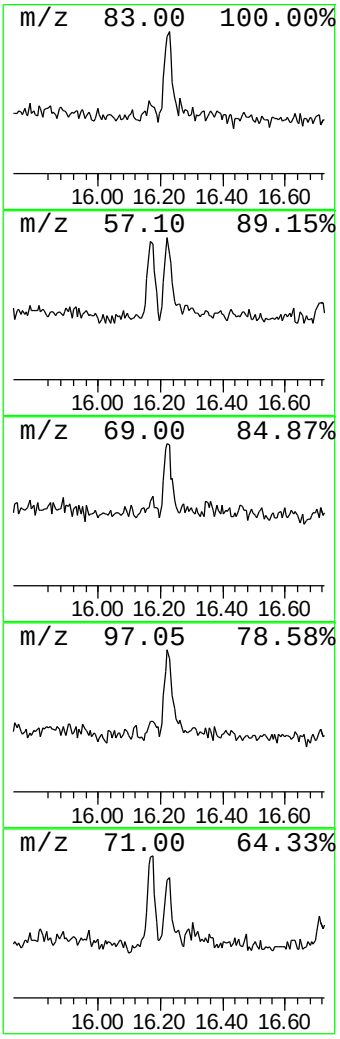
Peak Number 13 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	3.59 ng	133212	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	89
3	Octacosanol	410	C28H58O	000557-61-9	70
4	Octacosyl acetate	452	C30H60O2	018206-97-8	70
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	70





Tentatively Identified Compound (LSC) summary

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Operator : JU/SJ
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Misc :
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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...	2.33	4.1	ng	207239	1	6.97	1009490	20.0
2-Pentanone, 4-hy...	5.23	5.0	ng	252689	1	6.97	1009490	20.0
unknown6.75	6.75	88.6	ng	4470500	1	6.97	1009490	20.0
o-Toluidine	7.42	2.7	ng	136791	1	6.97	1009490	20.0
Tetradecane	10.90	2.9	ng	164503	4	11.50	1123780	20.0
p,p'-Ditolylamine	11.62	2.6	ng	143610	4	11.50	1123780	20.0
n-Hexadecanoic acid	12.02	4.7	ng	263260	4	11.50	1123780	20.0
1-Heneicosanol	13.97	10.6	ng	657291	5	14.16	1237610	20.0
1-Heptacosanol	14.62	2.5	ng	154445	5	14.16	1237610	20.0
Benzo[e]pyrene	15.56	3.1	ng	115681	6	15.70	742802	20.0
Cyclopentadecane	16.23	3.6	ng	133212	6	15.70	742802	20.0