LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100955.D
Acq On : 29 Nov 2017 1:43
Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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-BF110817.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	5.087	506	510	522	rBV	148053	193510	13.55%	1.310%
2	5.481	572	577	580	rBV	1407503	1344233	94.11%	9.103%
3	6.492	744	749	760	rBV	1329076	1342583	94.00%	9.092%
4	6.628	768	772	775	rBV	1483922	1382601	96.80%	9.363%
5	6.857	808	811	815	rBV	468923	357744	25.05%	2.423%
6	7.016	834	838	841	rBV	1291719	1081387	75.71%	7.323%
7	7.422	902	907	910	rBV	900240	806432	56.46%	5.461%
8	8.139	1025	1029	1032	rBV	540918	425886	29.82%	2.884%
9	8.692	1120	1123	1127	rBV	61813	48367	3.39%	0.328%
10	9.216	1207	1212	1215	rBV	1630224	1428334	100.00%	9.672%
11	9.604	1275	1278	1286	rVB	42576	33478	2.34%	0.227%
12	9.892	1323	1327	1331	rBV2	436365	393249	27.53%	2.663%
13	9.928	1331	1333	1337	rVB	20151	16723	1.17%	0.113%
14	10.604	1444	1448	1455	rBV	217283	178854	12.52%	1.211%
15	10.680	1458	1461	1469	rBV	711737	683612	47.86%	4.629%
16	11.380	1577	1580	1582	rBV	437614	353645	24.76%	2.395%
17	11.404	1582	1584	1588	rVV	193349	147112	10.30%	0.996%
18	11.457	1590	1593	1596	rVB	34921	27182	1.90%	0.184%
19	11.880	1662	1665	1666	rBV	24543	19280	1.35%	0.131%
20	11.910	1666	1670	1673	rVB2	37767	48791	3.42%	0.330%
21	11.992	1681	1684	1687	rBV	35857	42933	3.01%	0.291%
22	12.427	1755	1758	1761	rBV	16007	16876	1.18%	0.114%
23	12.516	1770	1773	1778	rVB2	16286	19969	1.40%	0.135%
24	12.592	1783	1786	1790	rBV	329158	287766	20.15%	1.949%
25	12.821	1819	1825	1829	rBV	317249	335633	23.50%	2.273%
26	12.874	1831	1834	1838	rVB2	14067	16412	1.15%	0.111%
27	12.963	1845	1849	1853	rBV	1298028	1179145	82.55%	7.985%
28	13.039	1856	1862	1867	rBV4	21602	37980	2.66%	0.257%
29	13.127	1874	1877	1878	rBV2	19566	19864	1.39%	0.135%
30	13.151	1878	1881	1884	rVB	38310	38159	2.67%	0.258%
31	13.216	1890	1892	1895	rBV	19784	16589	1.16%	0.112%
32	13.257	1895	1899	1901	rVV2	33794	35843	2.51%	0.243%
33	13.351	1912	1915	1917	rBV2	23006	20690	1.45%	0.140%
34	13.380	1917	1920	1923	rVB2	24287	24040	1.68%	0.163%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.657	1964	1967	1971	rVB	29000	27511	1.93%	0.186%
36	13.768	1981	1986	1989	rBV3	30191	43483	3.04%	0.294%
37	13.798	1989	1991	1993	rVV	34106	29089	2.04%	0.197%
38	13.821	1993	1995	1999	rVV2	27421	42724	2.99%	0.289%
39	13.863	1999	2002	2010	rVB3	58269	90707	6.35%	0.614%
40	14.021	2021	2029	2032	rBV2	540967	648630	45.41%	4.392%
41	14.045	2032	2033	2041	rVB	163430	132408	9.27%	0.897%
42	14.127	2045	2047	2052	rVB	25801	23848	1.67%	0.161%
43	14.410	2092	2095	2097	rVB	32785	28227	1.98%	0.191%
44	14.439	2098	2100	2103	rVB	22912	17699	1.24%	0.120%
45	14.533	2113	2116	2118	rBV2	24039	20992	1.47%	0.142%
46	15.063	2202	2206	2209	rBV	126297	182446	12.77%	1.235%
47	15.121	2213	2216	2221	rVB3	29544	41957	2.94%	0.284%
48	15.168	2221	2224	2227	rBV	21004	24102	1.69%	0.163%
49	15.368	2254	2258	2263	rVB	73836	93190	6.52%	0.631%
50	15.433	2264	2269	2273	rBV	97795	128785	9.02%	0.872%
51	15.498	2275	2280	2283	rBV	290796	363069	25.42%	2.459%
52	15.621	2298	2301	2304	rBV4	13960	17814	1.25%	0.121%
53	15.933	2350	2354	2359	rVB2	40346	55223	3.87%	0.374%
54	16.439	2435	2440	2445	rVB3	36515	57743	4.04%	0.391%
55	16.627	2467	2472	2478	rVB8	18551	38925	2.73%	0.264%
56	16.962	2526	2529	2536	rVB2	33056	57932	4.06%	0.392%
57	17.033	2536	2541	2546	rBV4	22530	44127	3.09%	0.299%
58	17.198	2567	2569	2573	rVB4	11568	16237	1.14%	0.110%
59	17.415	2601	2606	2614	rBV2	29867	59315	4.15%	0.402%
60	17.721	2653	2658	2664	rBV8	18342	40327	2.82%	0.273%
61	18.568	2796	2802	2811	rVB8	10145	35646	2.50%	0.241%

Sum of corrected areas: 14767058

LSC Report - Integrated Chromatogram

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Data File : BF100955.D
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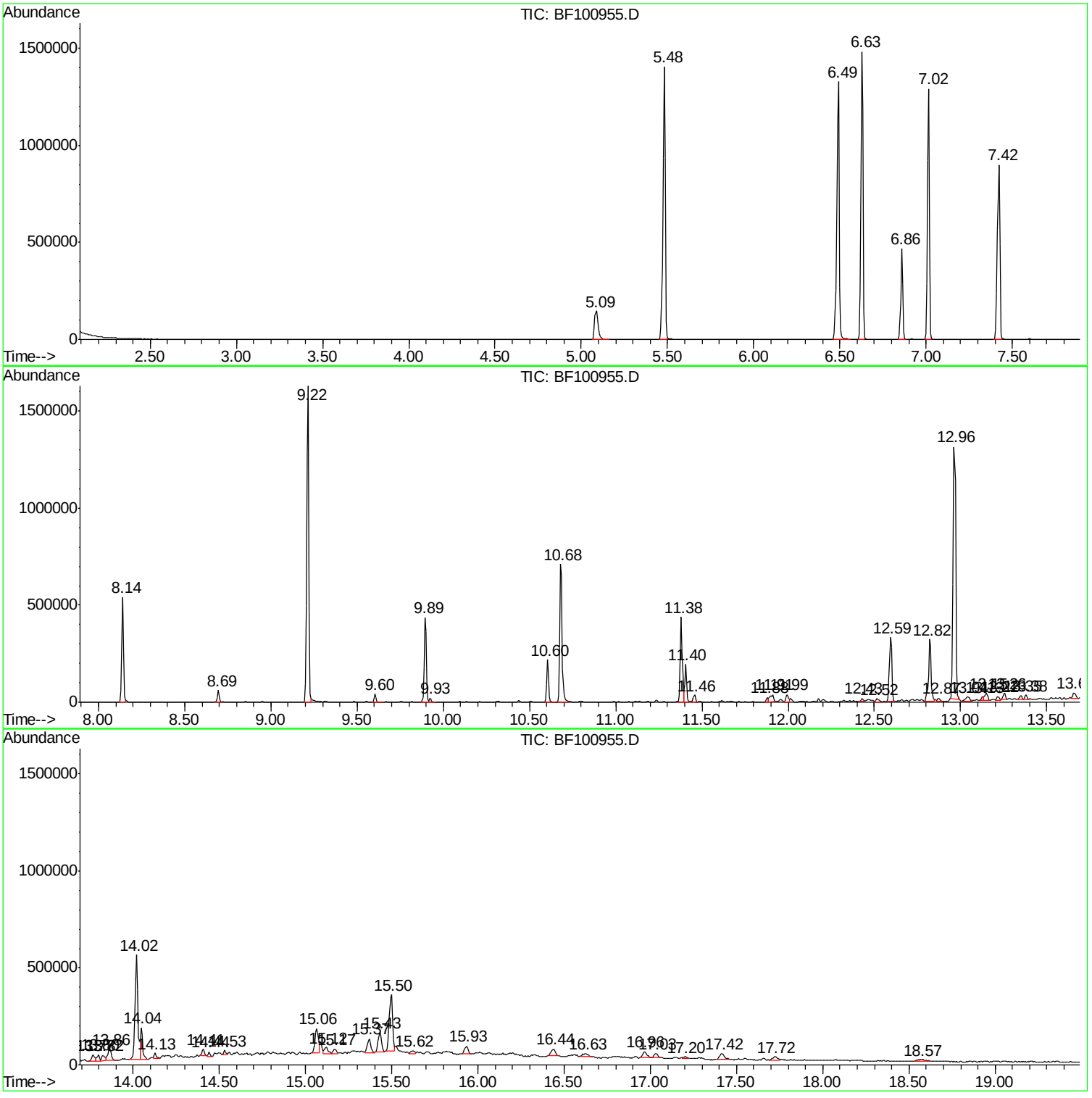
Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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\BF112817\
Data File : BF100955.D
Acq On : 29 Nov 2017 1:43
Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

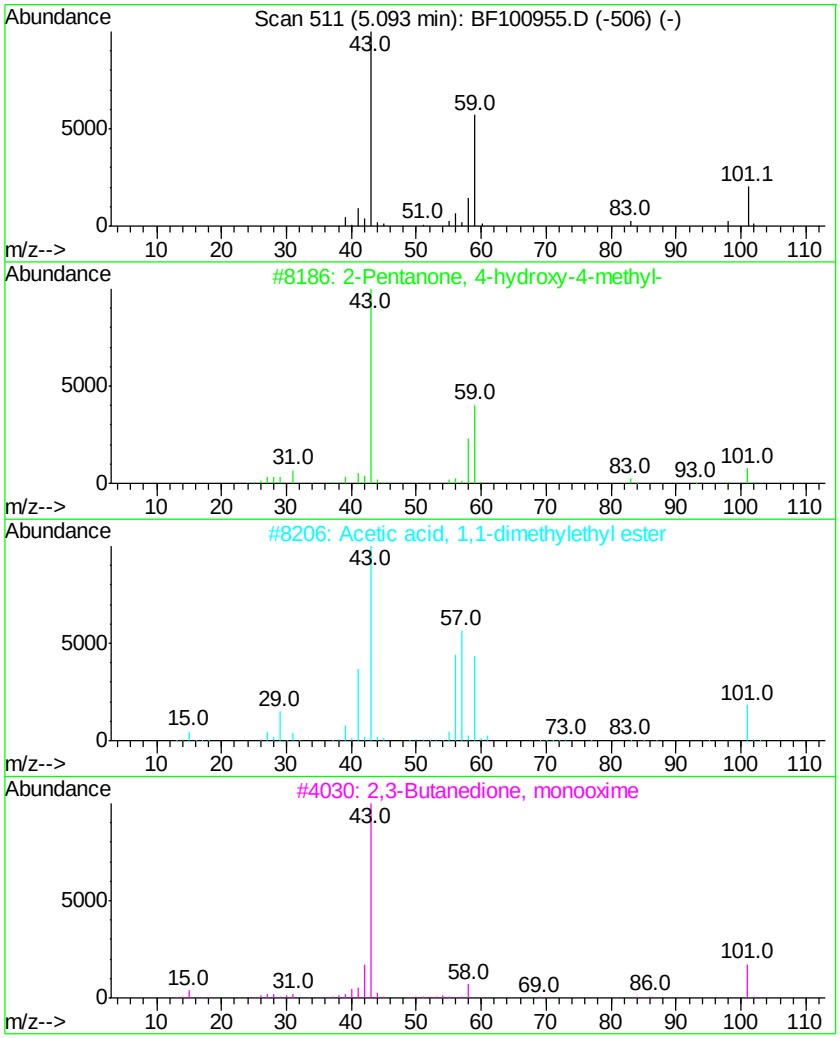
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

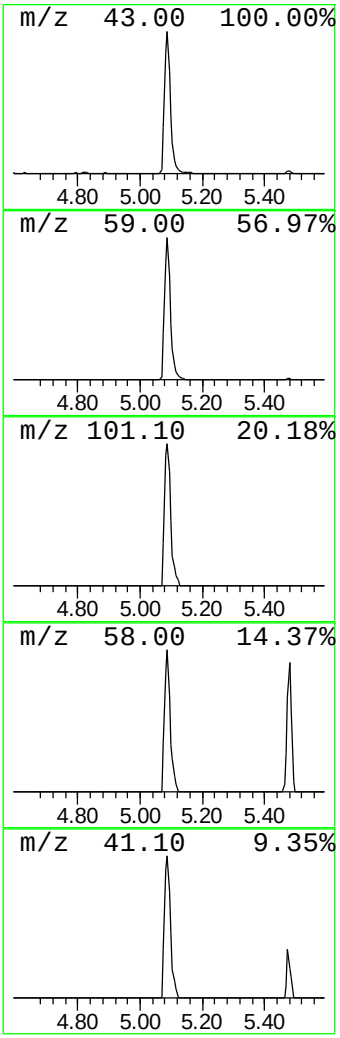
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	10.82 ng	193510	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
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Sample : I6579-07
Misc :
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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

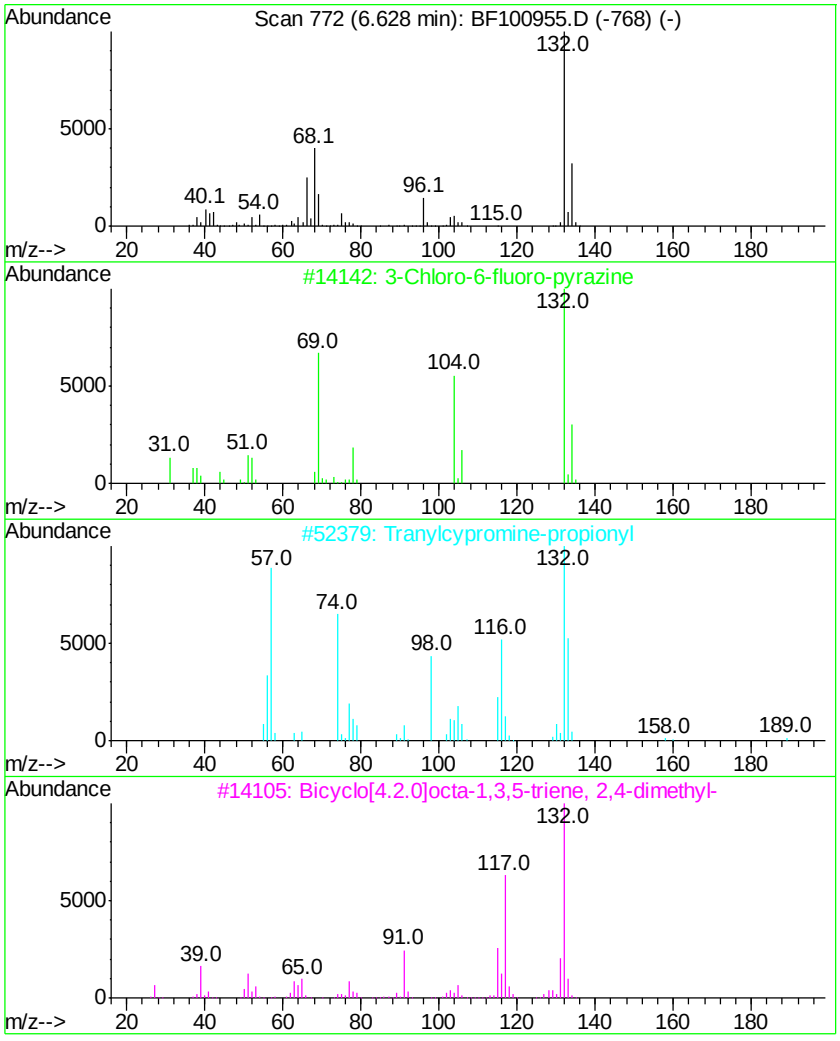
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

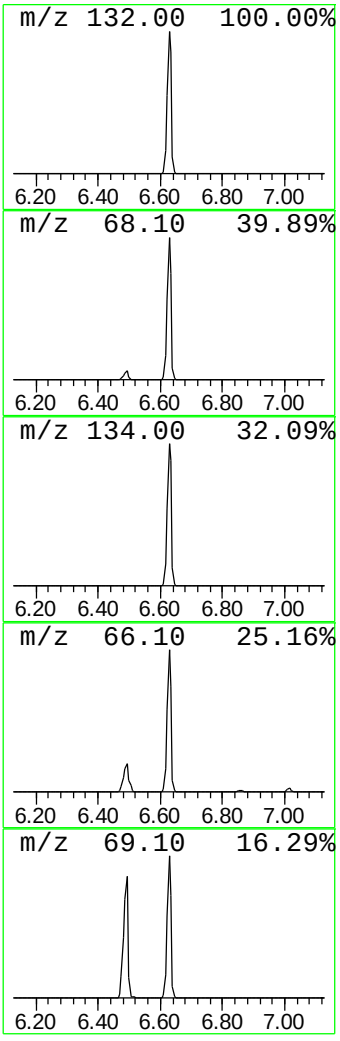
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	77.30 ng	1382600	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
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Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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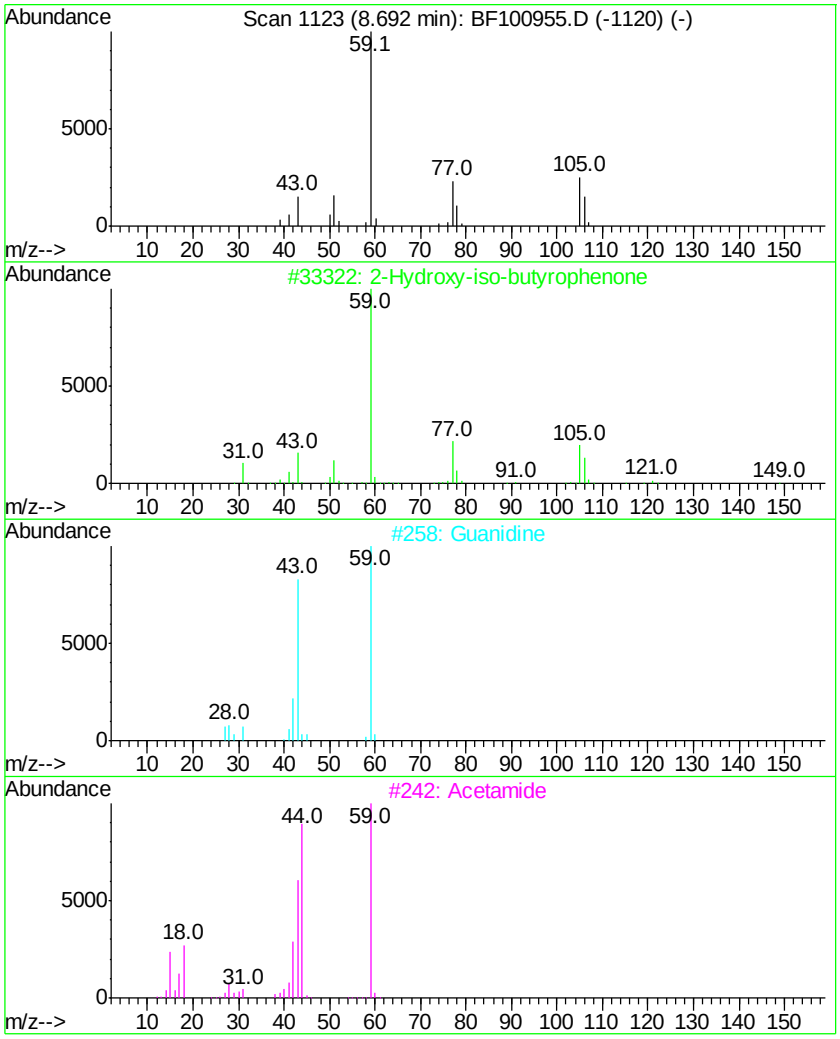
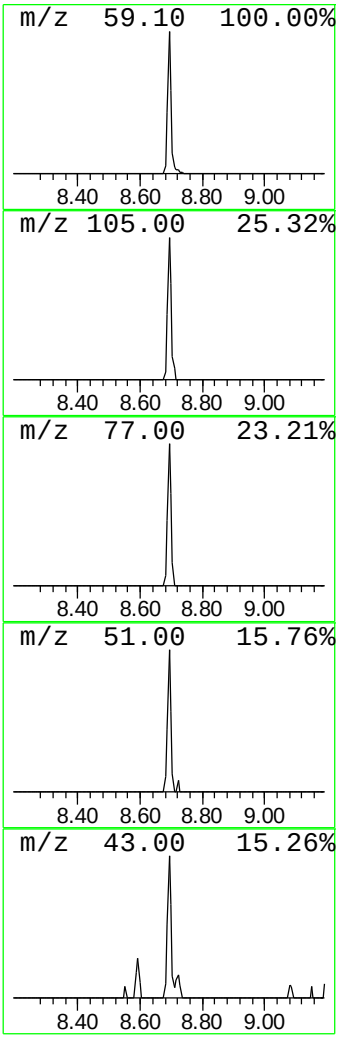
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	2.27 ng	48367	Naphthalene-d8	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Guanidine	59	CH5N3	000113-00-8	7
3	Acetamide	59	C2H5NO	000060-35-5	5
4	Propylamine	59	C3H9N	000107-10-8	4
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
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Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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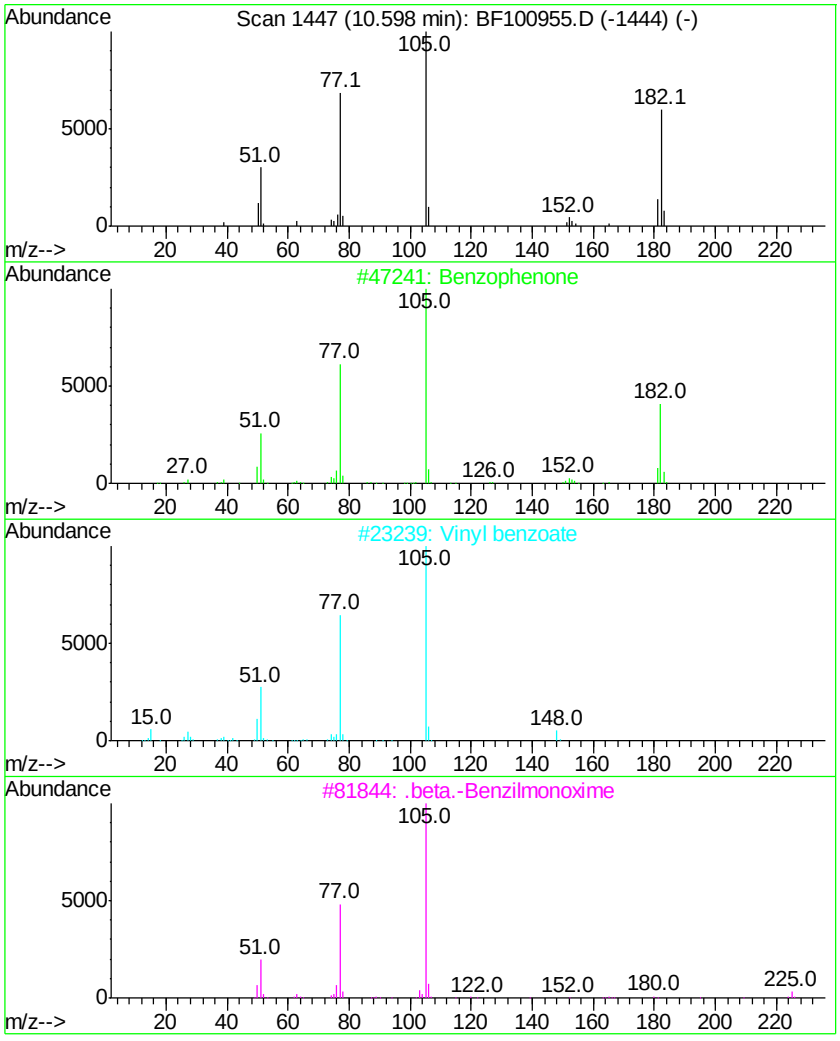
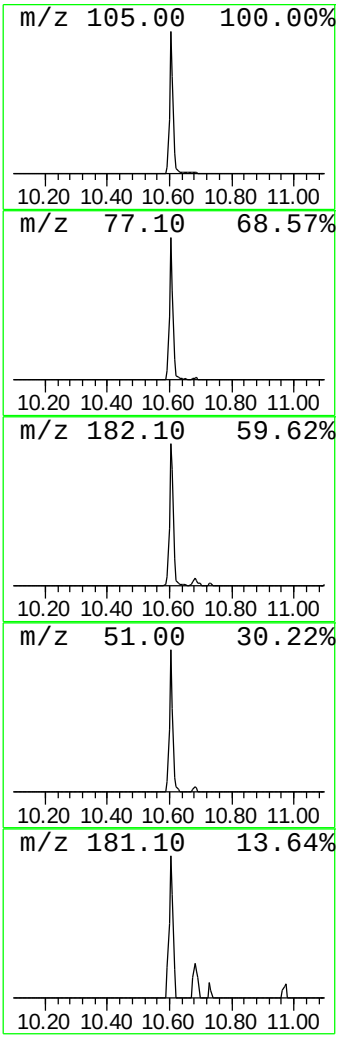
Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	9.10 ng	178854	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Vinyl benzoate	148	C9H8O2	000769-78-8	47
3	.beta.-Benzilmonoxime	225	C14H11NO2	014090-77-8	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	43





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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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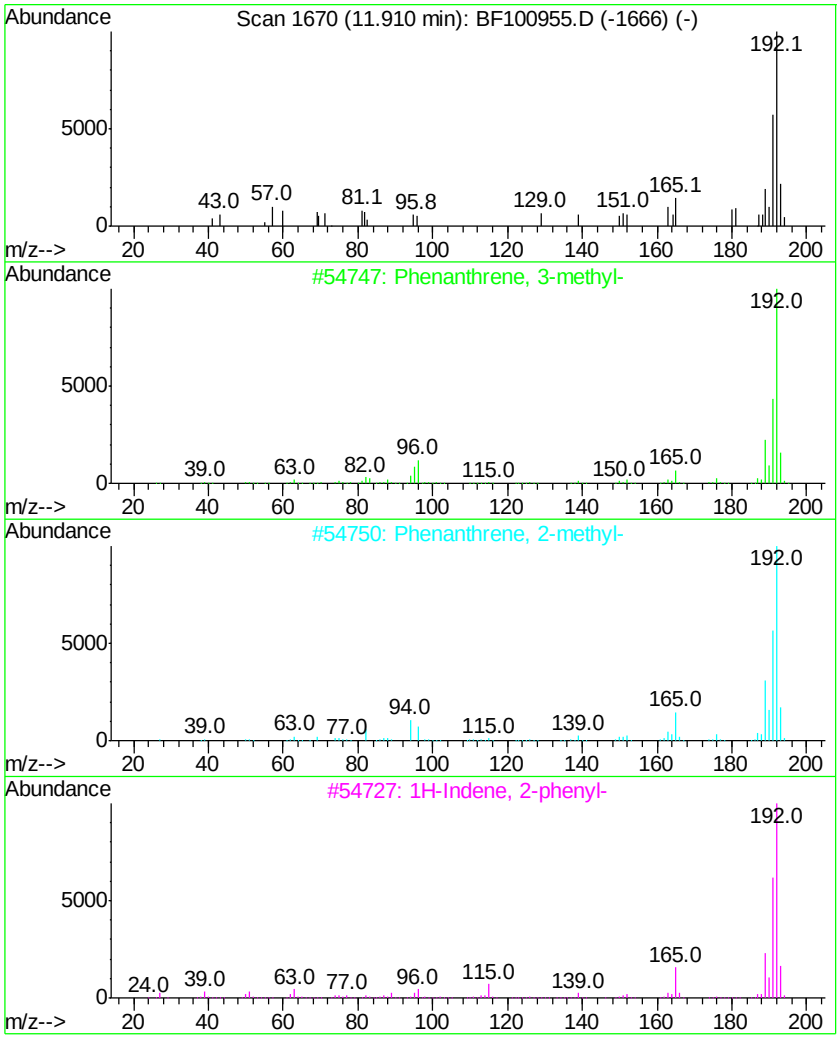
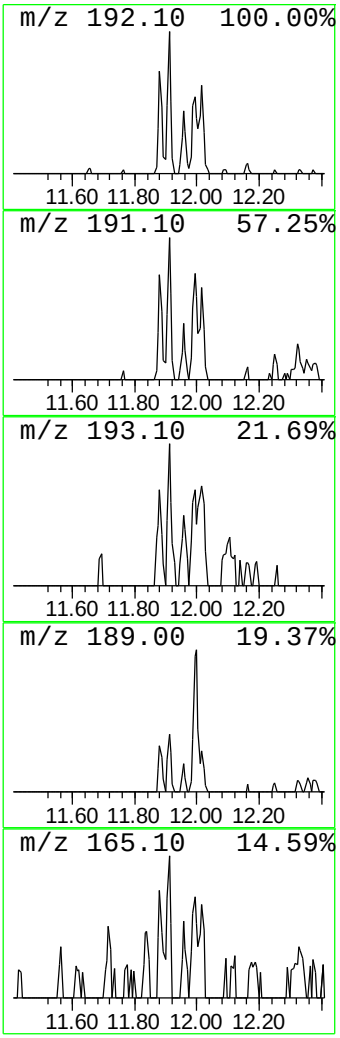
Peak Number 6 Phenanthrene, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.76 ng	48791	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	76
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	74
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	72
4	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	72
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	68





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Sample : I6579-07
Misc :
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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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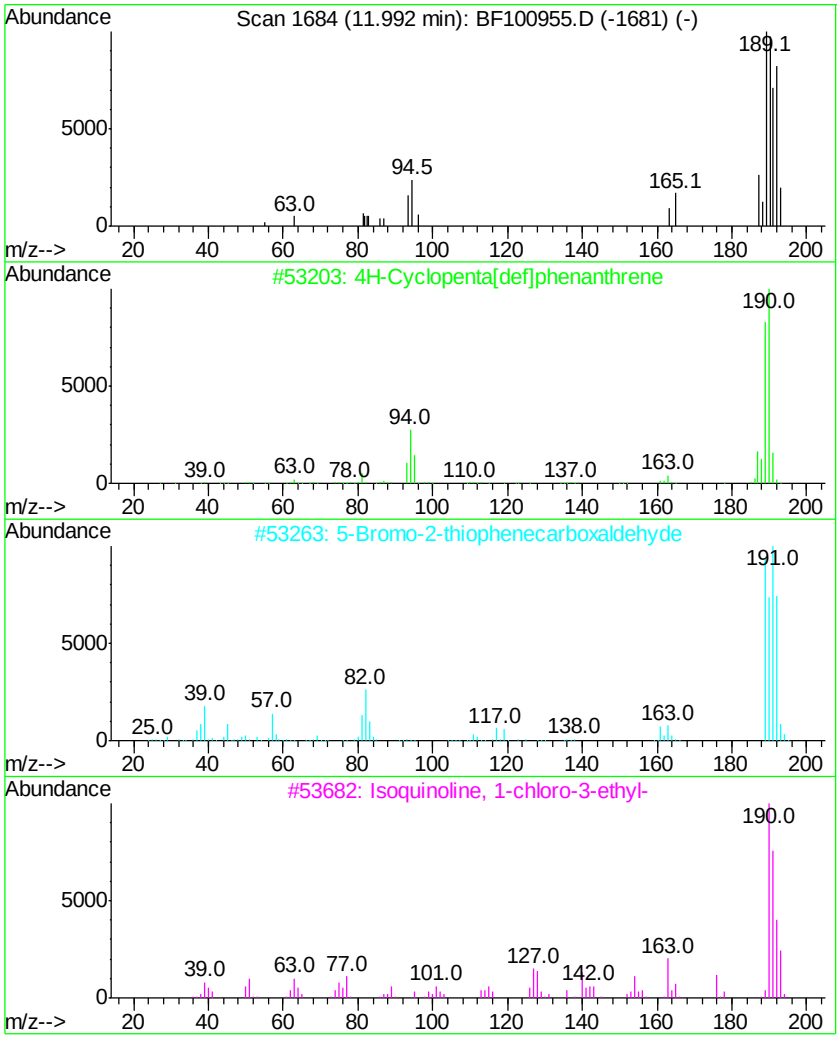
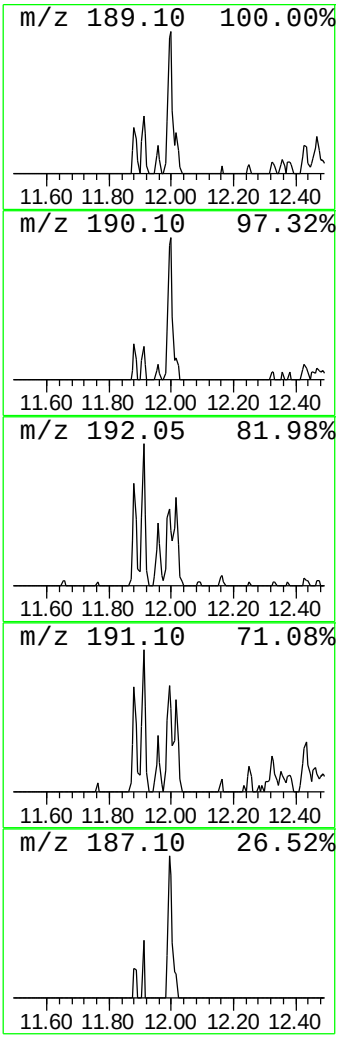
Peak Number 7 unknown11.99 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.43 ng	42933	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
2	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	42
3	Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	38
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	32





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Operator : SJ/JU
Sample : I6579-07
Misc :
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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

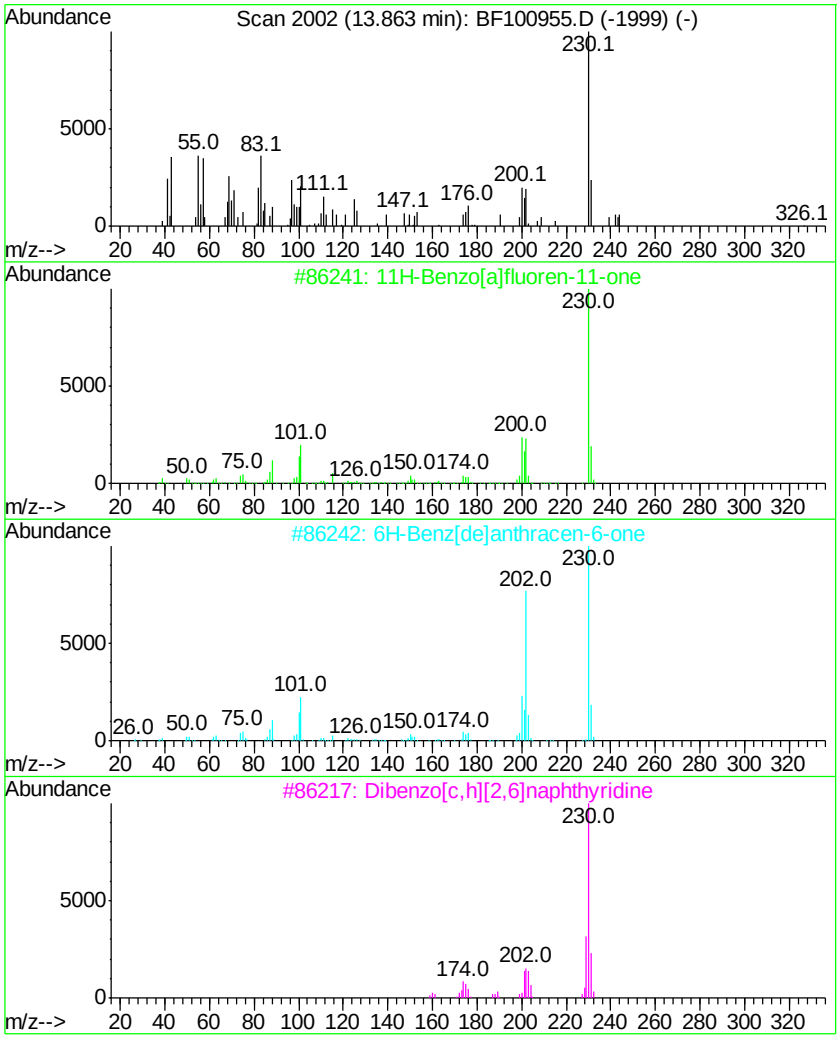
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

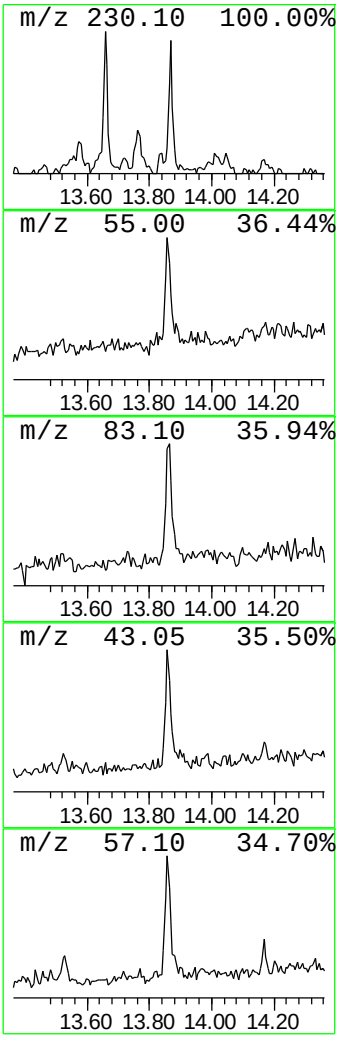
****

Peak Number 8 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.80 ng	90707	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	81
2	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	70
3	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	59
4	(E)-.alpha.,.alpha.'-Dicyanostil...	230	C16H10N2	002450-55-7	52
5	Naphthalene, 2-styryl-	230	C18H14	002039-70-5	50





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Data File : BF100955.D
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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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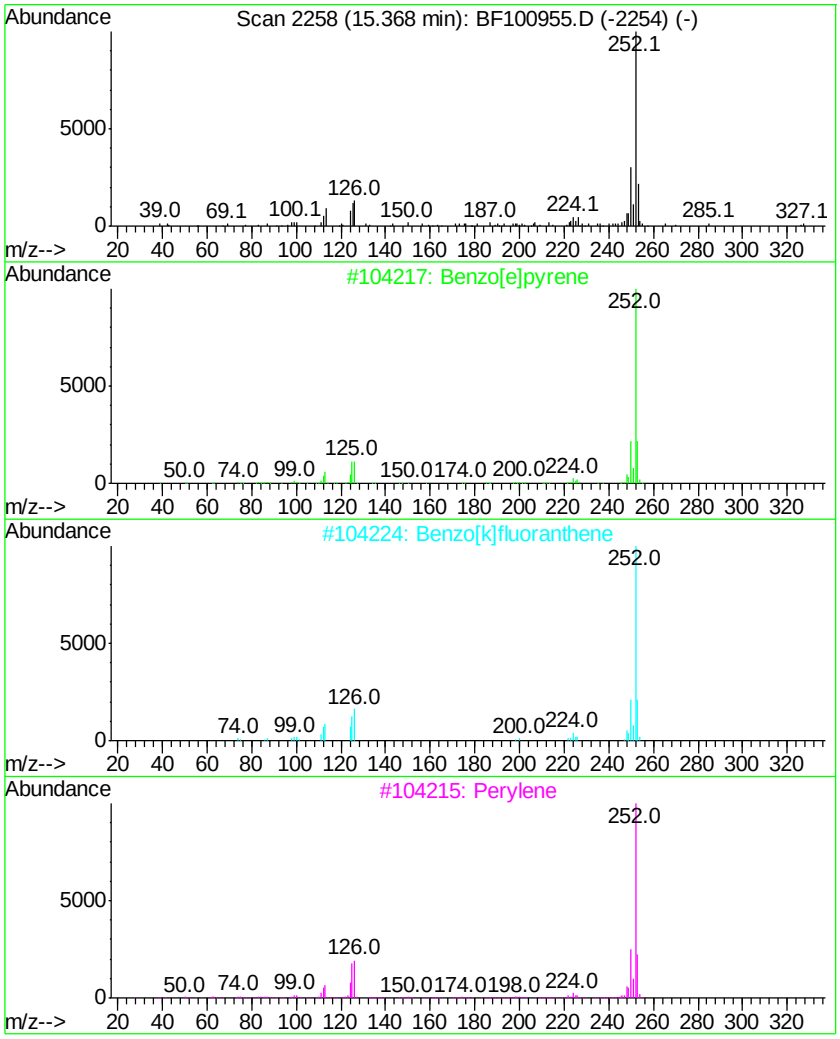
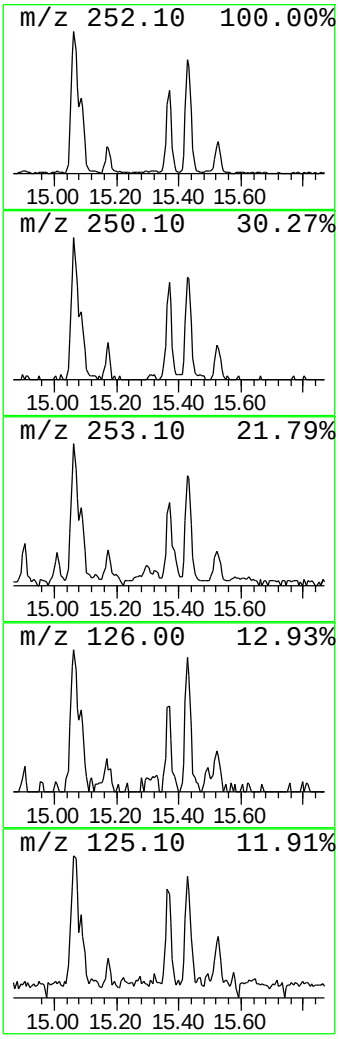
Peak Number 9 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	5.13 ng	93190	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Perylene	252	C20H12	000198-55-0	94
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	91





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Data File : BF100955.D
Acq On : 29 Nov 2017 1:43
Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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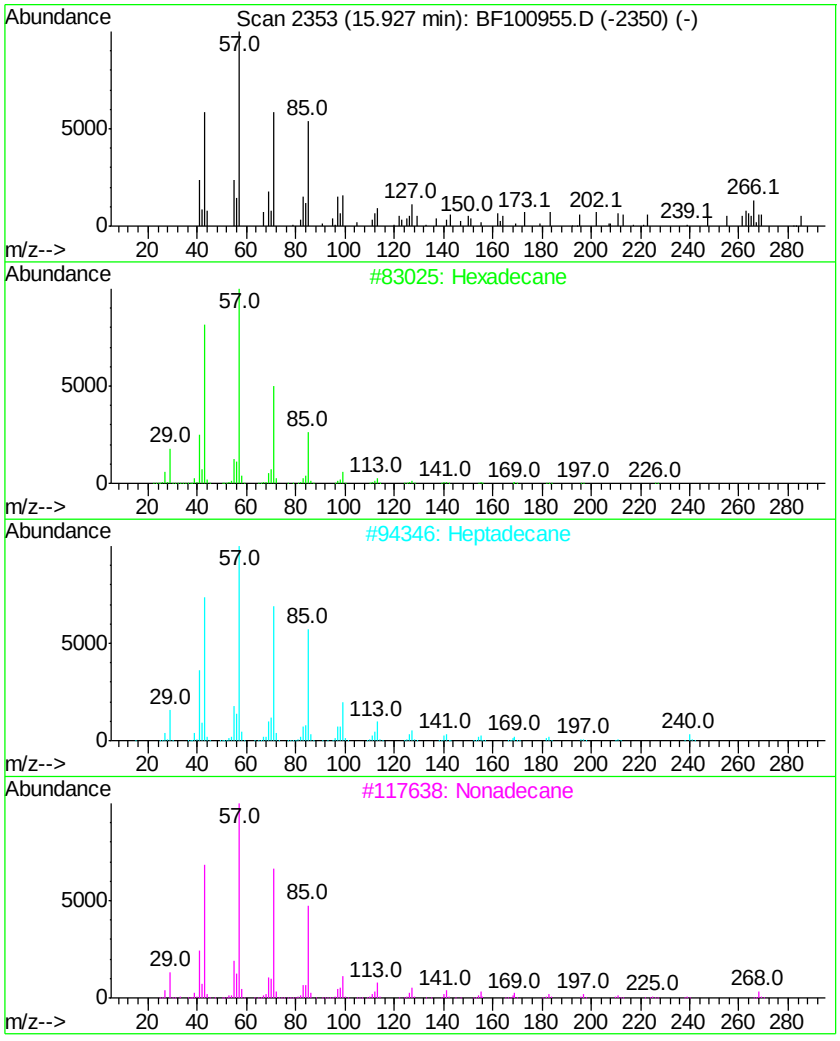
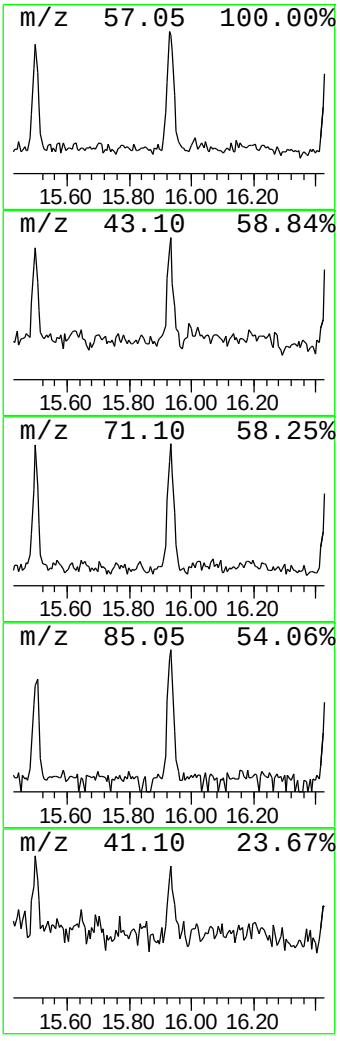
Peak Number 10 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.04 ng	55223	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptadecane	240	C17H36	000629-78-7	83
3	Nonadecane	268	C19H40	000629-92-5	83
4	Pentadecane	212	C15H32	000629-62-9	49
5	Hexacosane	366	C26H54	000630-01-3	49





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Operator : SJ/JU
Sample : I6579-07
Misc :
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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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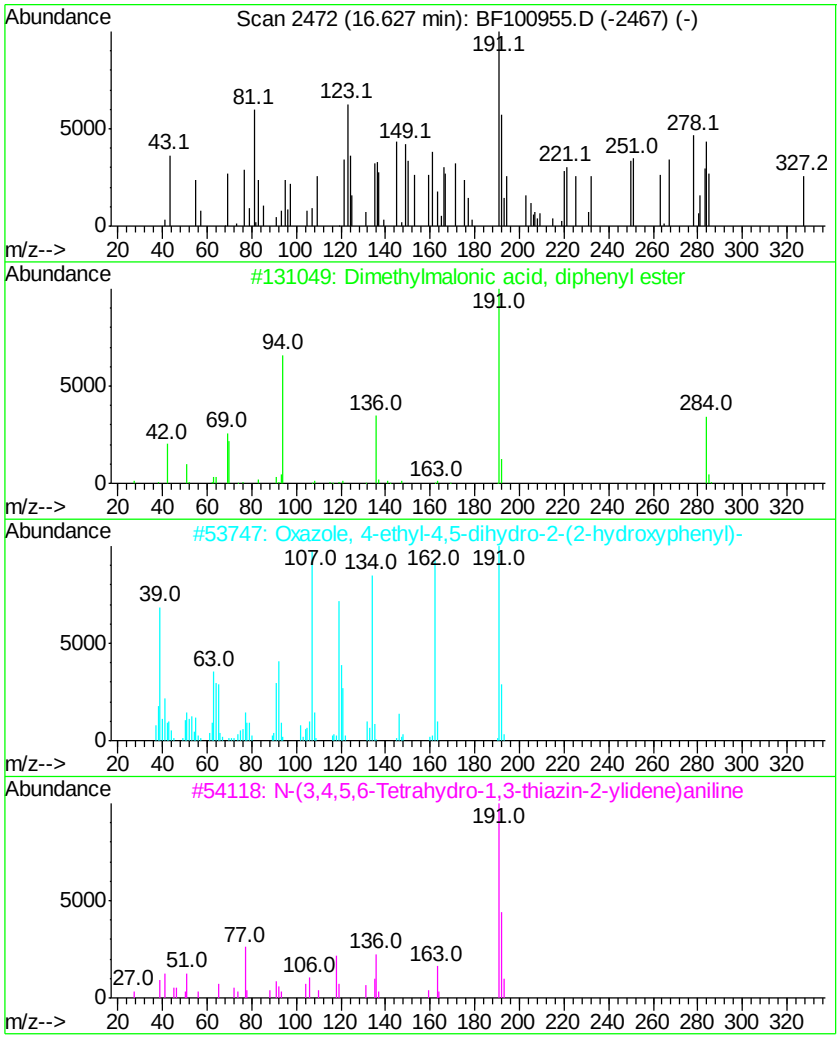
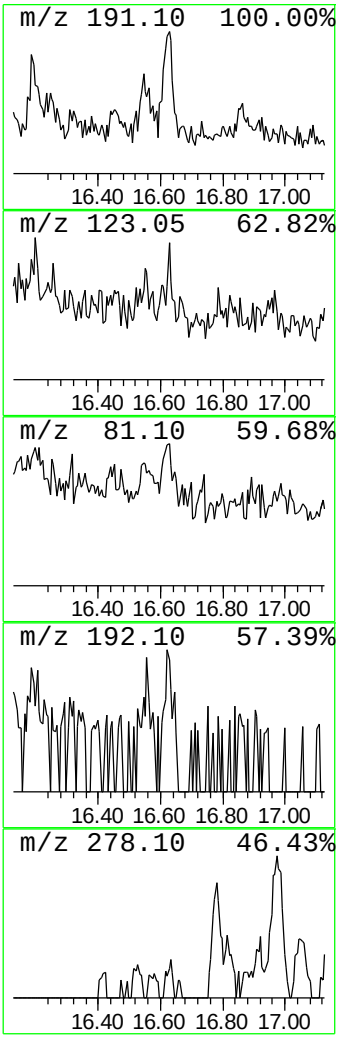
Peak Number 12 unknown16.63 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.14 ng	38925	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethylmalonic acid, diphenyl e...	284	C17H16O4	1000361-81-0	30
2	Oxazole, 4-ethyl-4,5-dihydro-2-(...	191	C11H13NO2	1000142-01-8	25
3	N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	25
4	N-[4-(Acetylamino)tricyclo[3.3.1...	250	C14H22N2O2	1000305-58-9	25
5	N,N'-di-sec-Butyl-p-phenylenedia...	220	C14H24N2	000101-96-2	14





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Operator : SJ/JU
Sample : I6579-07
Misc :
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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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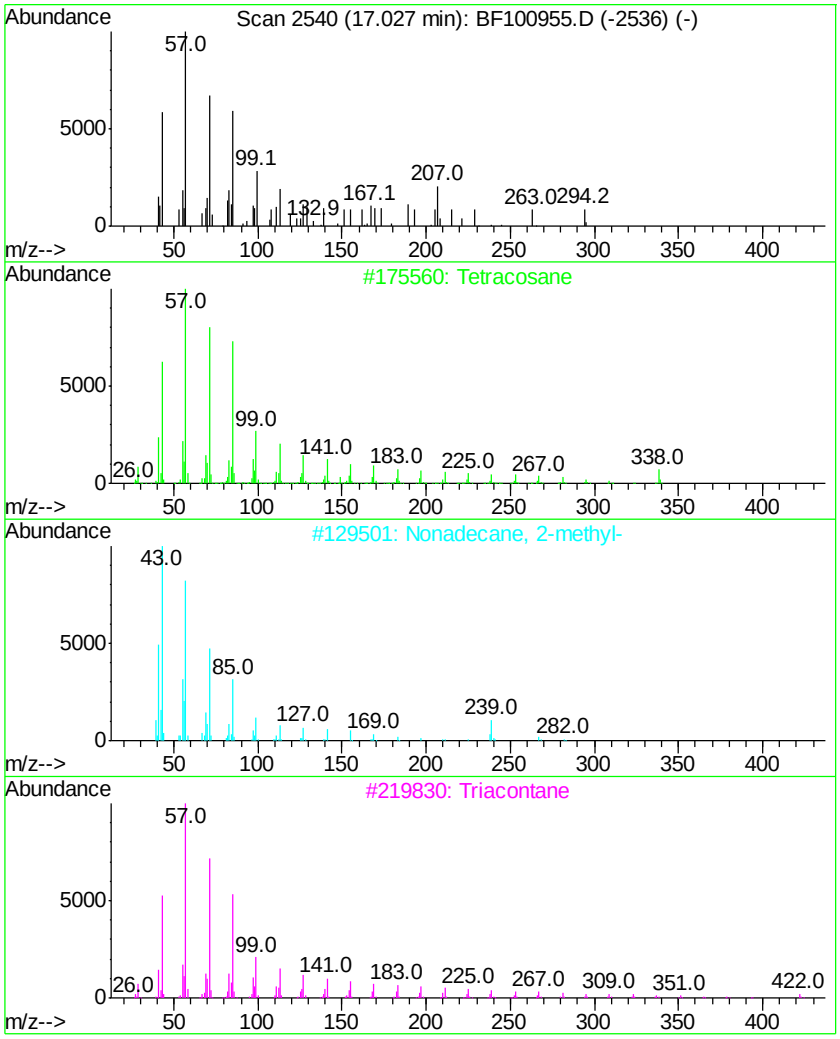
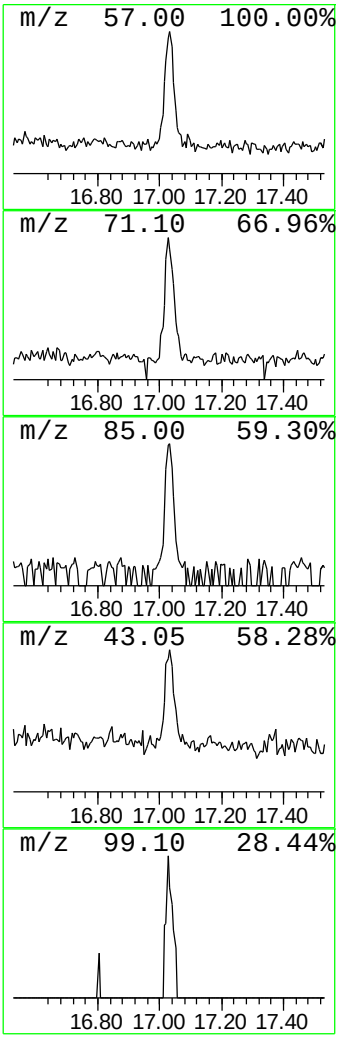
Peak Number 13 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	2.43 ng	44127	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	64
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	64
3	Triacontane	422	C30H62	000638-68-6	59
4	Docosane	310	C22H46	000629-97-0	53
5	Octadecane	254	C18H38	000593-45-3	50





Library Search Compound Report

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Data File : BF100955.D
Acq On : 29 Nov 2017 1:43
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Sample : I6579-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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TIC Integration Parameters: LSCINT.P

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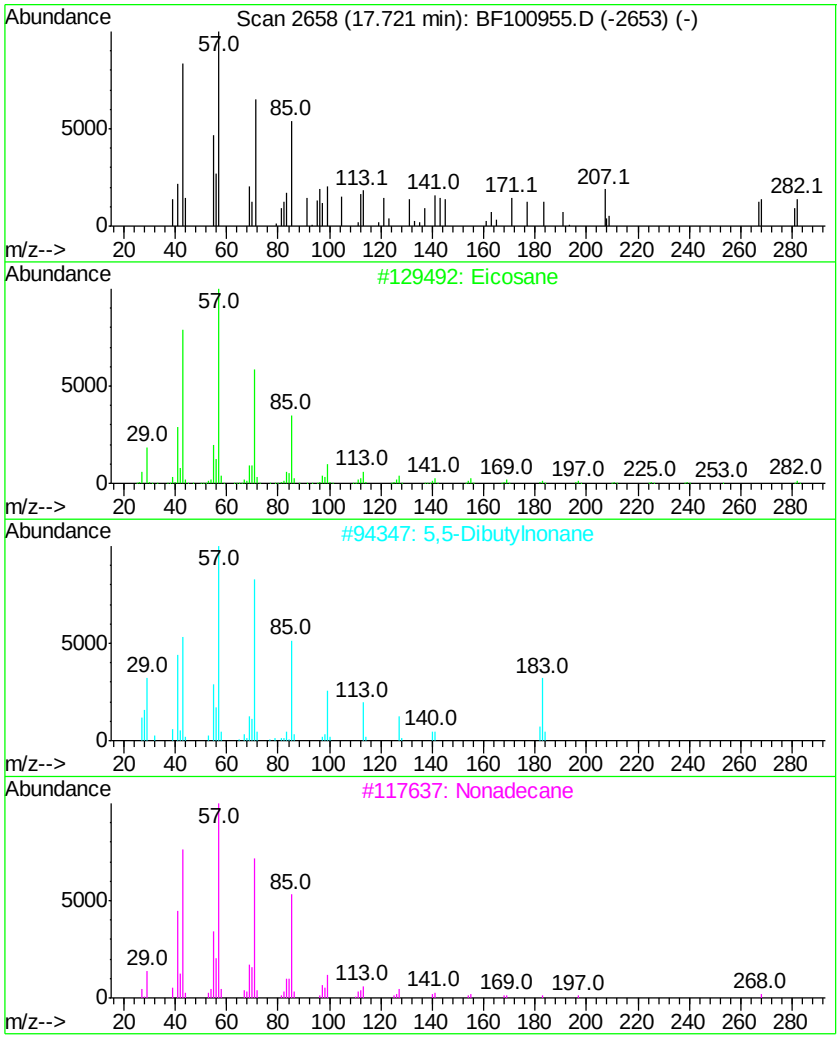
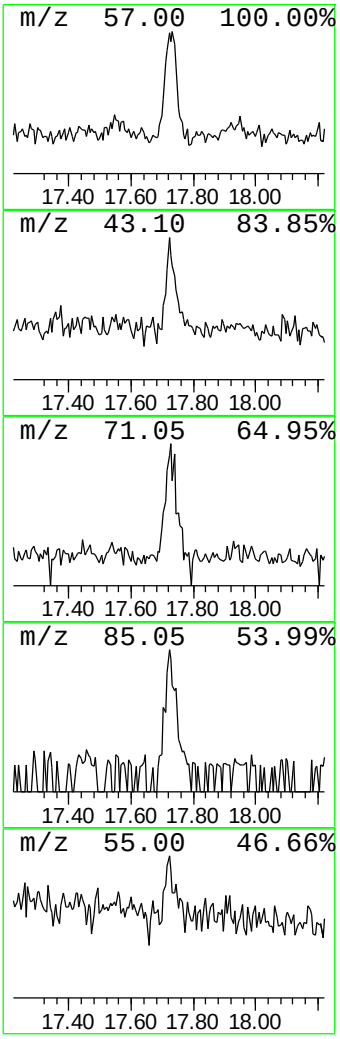
Peak Number 14 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.72	2.22 ng	40327	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	50
2	5,5-Dibutylnonane	240	C17H36	006008-17-9	47
3	Nonadecane	268	C19H40	000629-92-5	46
4	2-methyltetracosane	352	C25H52	1000376-72-6	46
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	43





Tentatively Identified Compound (LSC) summary

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Data File : BF100955.D
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Operator : SJ/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	10.8	ng	193510	1	6.86	357744	20.0
unknown6.63	6.63	77.3	ng	1382600	1	6.86	357744	20.0
2-Hydroxy-iso-but...	8.69	2.3	ng	48367	2	8.14	425886	20.0
Benzophenone	10.60	9.1	ng	178854	3	9.89	393249	20.0
Phenanthrene, 3-m...	11.91	2.8	ng	48791	4	11.38	353645	20.0
unknown11.99	11.99	2.4	ng	42933	4	11.38	353645	20.0
11H-Benzo[a]fluor...	13.86	2.8	ng	90707	5	14.02	648630	20.0
Benzo[e]pyrene	15.37	5.1	ng	93190	6	15.50	363069	20.0
Hexadecane	15.93	3.0	ng	55223	6	15.50	363069	20.0
unknown16.63	16.63	2.1	ng	38925	6	15.50	363069	20.0
Tetracosane	17.03	2.4	ng	44127	6	15.50	363069	20.0
Eicosane	17.72	2.2	ng	40327	6	15.50	363069	20.0