LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124202.D
Acq On : 9 Jun 2021 3:17
Operator : JU/CG
Sample : M2589-18 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(0-2)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124202.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.440	396	400	407	rBB	86288	100103	39.45%	5.111%
2	5.063	503	506	513	rBB	85230	78276	30.85%	3.996%
3	6.516	751	753	757	rBV	8517	7640	3.01%	0.390%
4	6.863	809	812	816	rBV	260811	200442	78.99%	10.234%
5	7.422	904	907	912	rBB	28489	22459	8.85%	1.147%
6	8.145	1027	1030	1034	rBV	267619	217722	85.80%	11.116%
7	9.222	1210	1213	1219	rVB	50978	41202	16.24%	2.104%
8	9.904	1325	1329	1337	rBB	309119	240152	94.63%	12.261%
9	10.816	1480	1484	1486	rBB	3469	4102	1.62%	0.209%
10	11.392	1578	1582	1585	rBV	320407	248680	98.00%	12.696%
11	11.416	1585	1586	1589	rVB	9109	5072	2.00%	0.259%
12	11.451	1589	1592	1596	rBV3	2918	3217	1.27%	0.164%
13	11.504	1600	1601	1605	rBV	2866	3104	1.22%	0.158%
14	11.892	1663	1667	1670	rVB3	2186	3164	1.25%	0.162%
15	11.939	1670	1675	1677	rBV2	2815	3777	1.49%	0.193%
16	11.992	1680	1684	1686	rBV	2649	3738	1.47%	0.191%
17	12.092	1698	1701	1702	rBV	2939	3251	1.28%	0.166%
18	12.127	1705	1707	1709	rVB3	5876	3848	1.52%	0.196%
19	12.157	1709	1712	1714	rBV2	5260	3654	1.44%	0.187%
20	12.345	1742	1744	1747	rVB3	4059	3743	1.47%	0.191%
21	12.439	1759	1760	1764	rBV3	4526	4329	1.71%	0.221%
22	12.480	1764	1767	1770	rBV5	4324	6584	2.59%	0.336%
23	12.516	1770	1773	1775	rVB3	3341	4227	1.67%	0.216%
24	12.557	1777	1780	1781	rBV2	4760	5012	1.98%	0.256%
25	12.610	1786	1789	1792	rVV2	13289	13753	5.42%	0.702%
26	12.692	1801	1803	1806	rBV2	2826	3368	1.33%	0.172%
27	12.739	1809	1811	1812	rBV	4119	3197	1.26%	0.163%
28	12.839	1824	1828	1831	rBV2	14951	16883	6.65%	0.862%
29	12.886	1834	1836	1838	rBV3	7532	5561	2.19%	0.284%
30	12.939	1843	1845	1848	rBV4	5676	7963	3.14%	0.407%
31	12.974	1848	1851	1855	rVB	64997	55539	21.89%	2.836%
32	13.027	1858	1860	1861	rBV2	7378	3932	1.55%	0.201%
33	13.068	1865	1867	1872	rBV5	4258	6285	2.48%	0.321%
34	13.110	1872	1874	1876	rBV3	6243	5564	2.19%	0.284%
35	13.157	1881	1882	1885	rBV3	8393	7189	2.83%	0.367%
36	13.345	1913	1914	1916	rBV2	7324	5640	2.22%	0.288%

LSC Area Percent Report

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Operator : JU/CG
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(0-2)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.457	1931	1933	1935	rVB3	12678	10308	4.06%	0.526%
38	13.486	1935	1938	1940	rBV4	7051	9859	3.89%	0.503%
39	13.539	1945	1947	1948	rBV2	6234	3805	1.50%	0.194%
40	13.568	1951	1952	1954	rBV2	7351	7301	2.88%	0.373%
41	13.704	1974	1975	1976	rBV	8377	4133	1.63%	0.211%
42	13.739	1979	1981	1982	rBV2	12048	8444	3.33%	0.431%
43	13.774	1985	1987	1988	rBV2	11962	7151	2.82%	0.365%
44	13.792	1988	1990	1991	rVB2	13545	6588	2.60%	0.336%
45	13.810	1991	1993	1994	rBV2	8289	6455	2.54%	0.330%
46	13.892	2006	2007	2010	rBV3	13850	15234	6.00%	0.778%
47	14.039	2028	2032	2035	rBV	250440	253768	100.00%	12.956%
48	14.145	2048	2050	2052	rBV3	13760	16831	6.63%	0.859%
49	15.198	2227	2229	2231	rBV3	28053	25169	9.92%	1.285%
50	15.527	2281	2285	2291	rVB	151838	200877	79.16%	10.256%
51	16.645	2473	2475	2479	rBV5	23486	30379	11.97%	1.551%

Sum of corrected areas: 1958674

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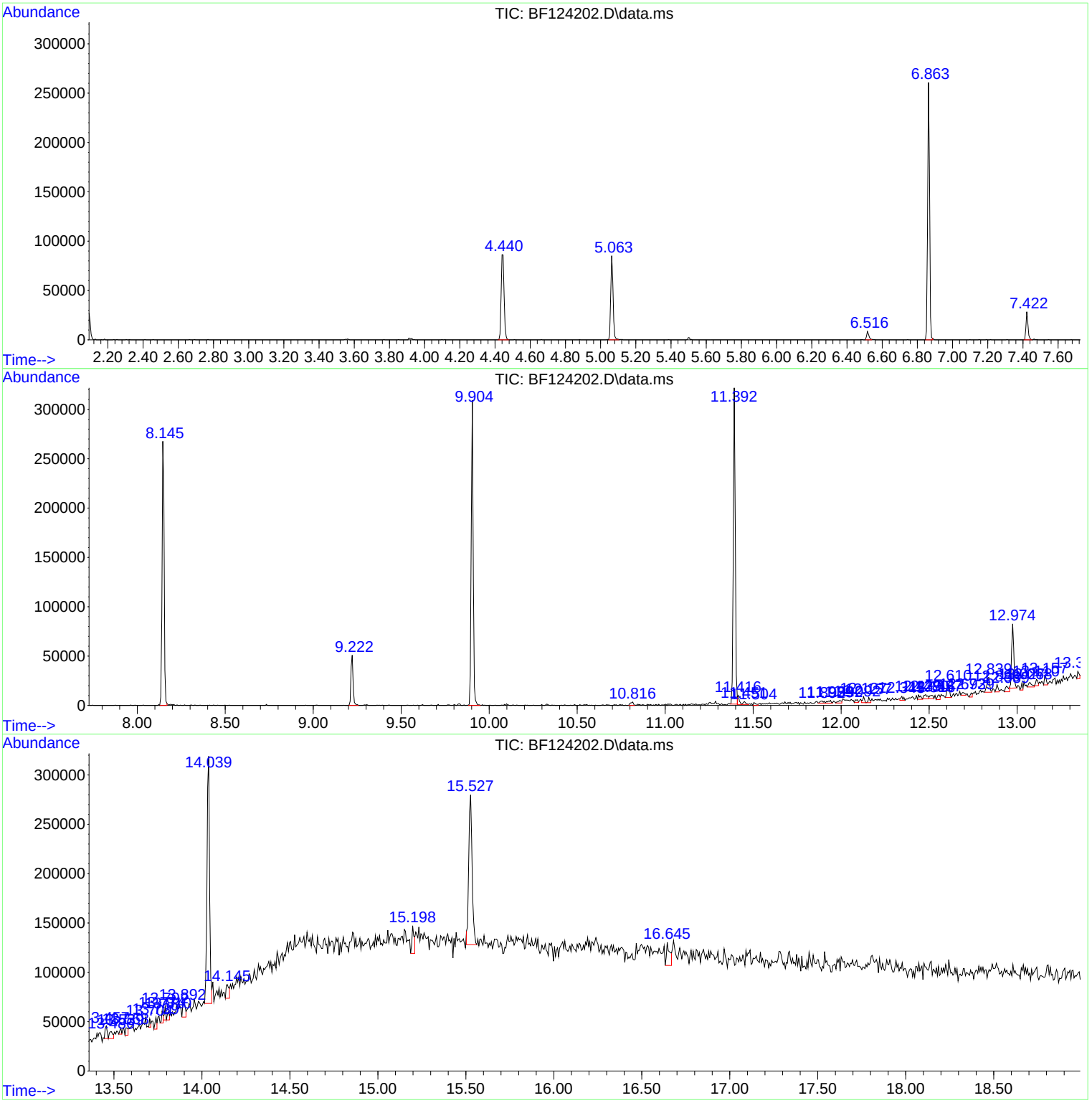
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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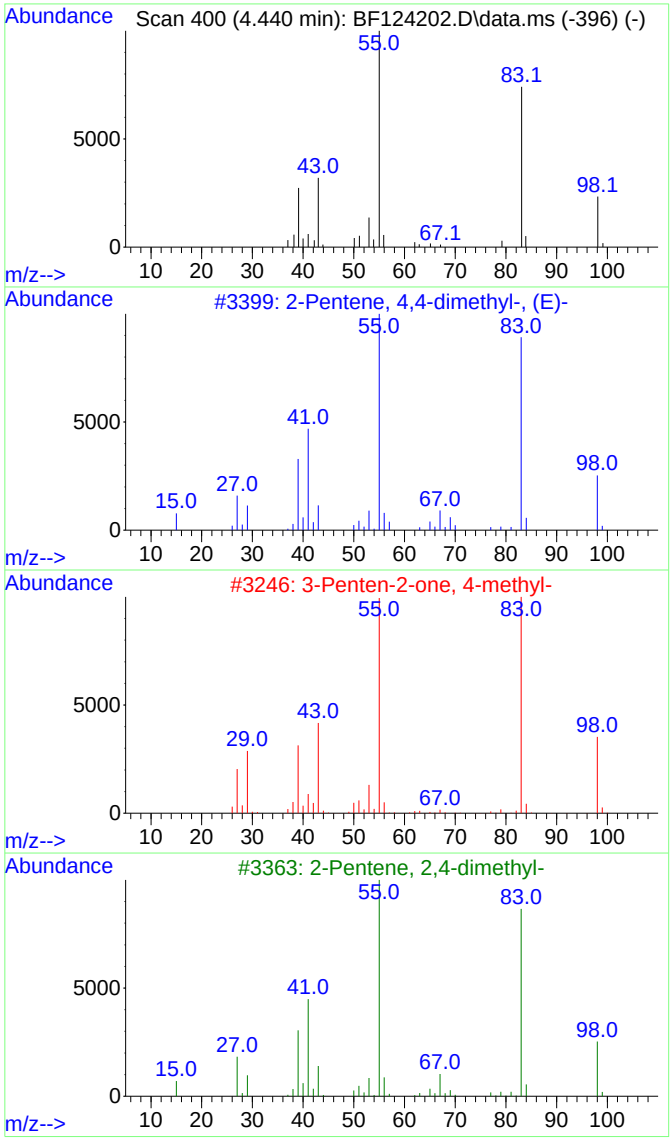
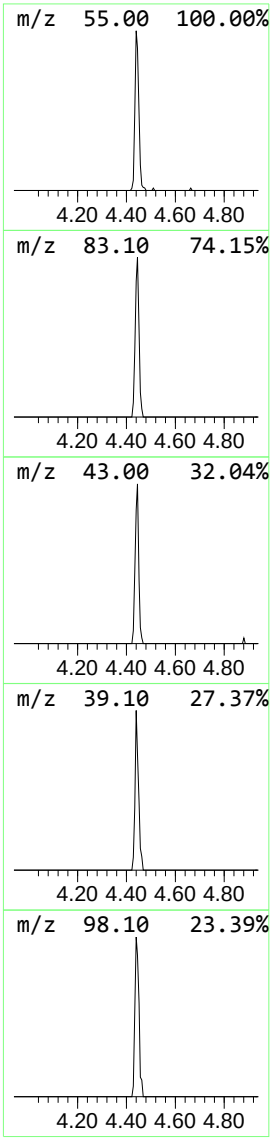
****

Peak Number 1 2-Pentene, 4,4-dimethyl-, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.440	9.99 ng	100103	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	90
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80





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Instrument :
BNA_F
ClientSampleId :
18-B12(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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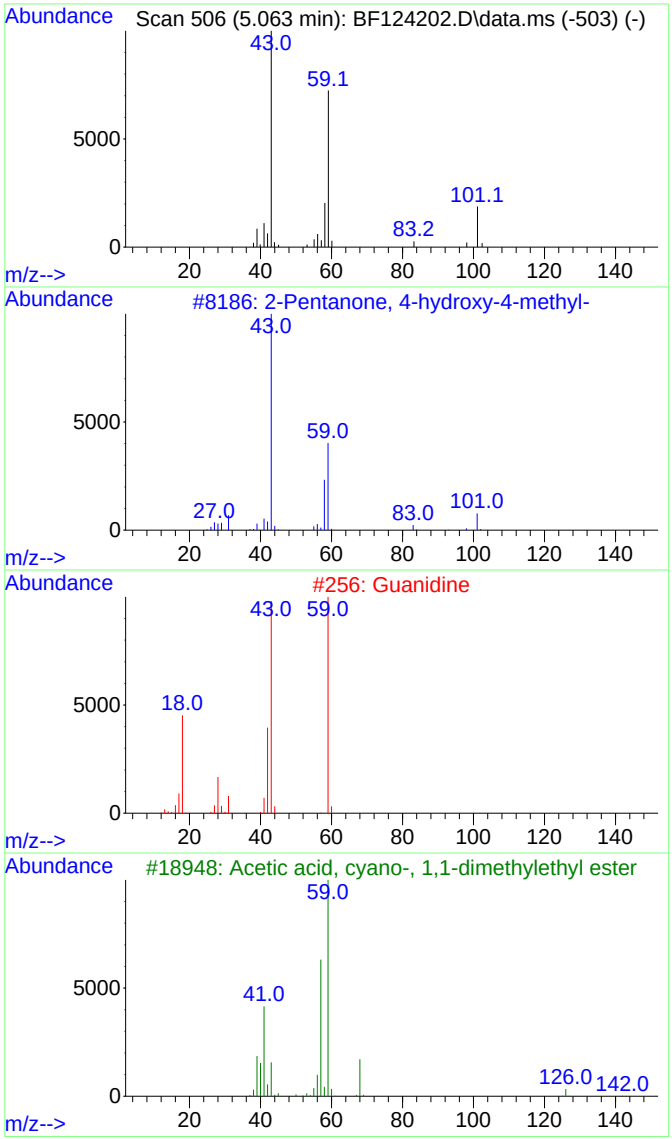
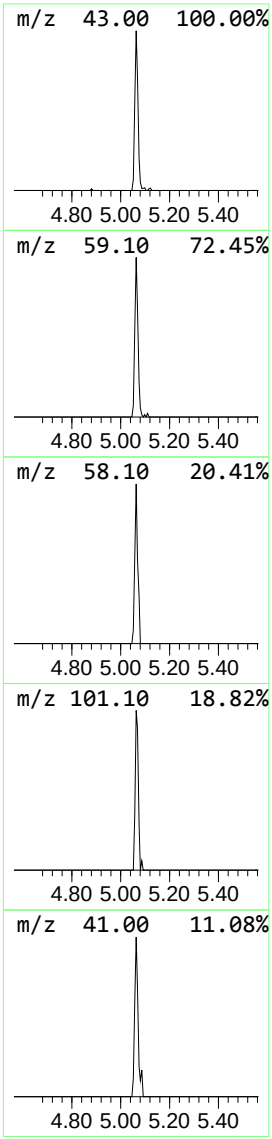
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	7.81 ng	78276	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Guanidine	59	CH5N3	000113-00-8	37
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	3-Octanol	130	C8H18O	000589-98-0	25
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23





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Instrument :
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ClientSampleId :
18-B12(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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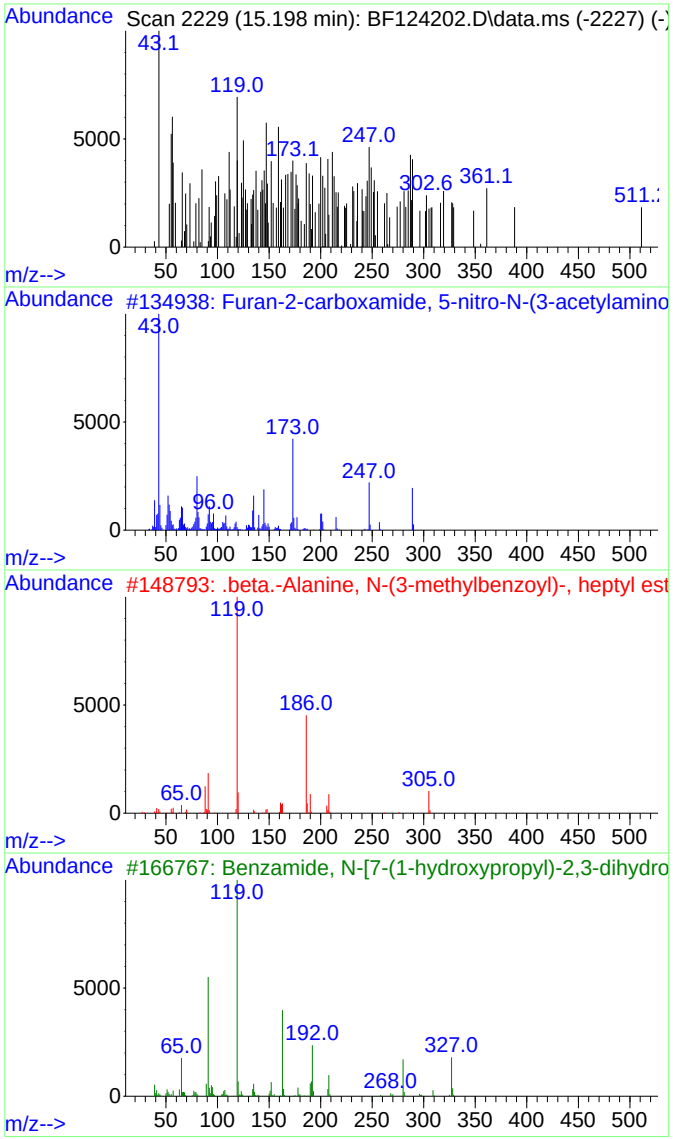
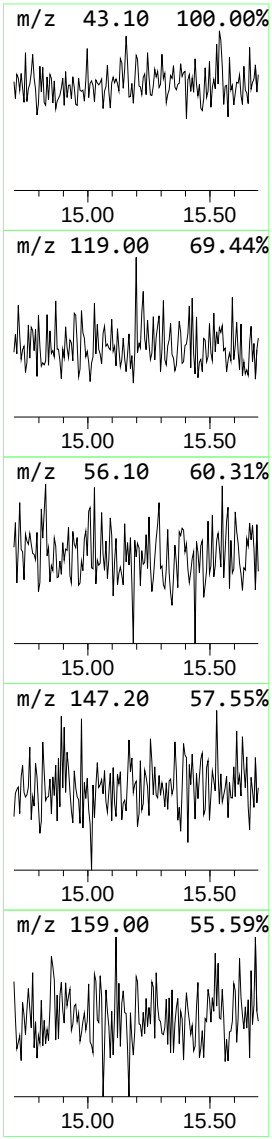
Peak Number 3 unknown15.198 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	2.51 ng	25169	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan-2-carboxamide, 5-nitro-N-(...	289	C13H11N3O5	299968-62-0	16
2	.beta.-Alanine, N-(3-methylbenzo...	305	C18H27NO3	1000321-63-0	14
3	Benzamide, N-[7-(1-hydroxypropyl...	327	C19H21NO4	1000316-96-2	11
4	Ethanone, 1-[4-(hydroxymethyl)-2...	247	C13H13NO2S	067387-03-5	10
5	Ethyl o-acetamidobenzoate	207	C11H13NO3	020628-20-0	10





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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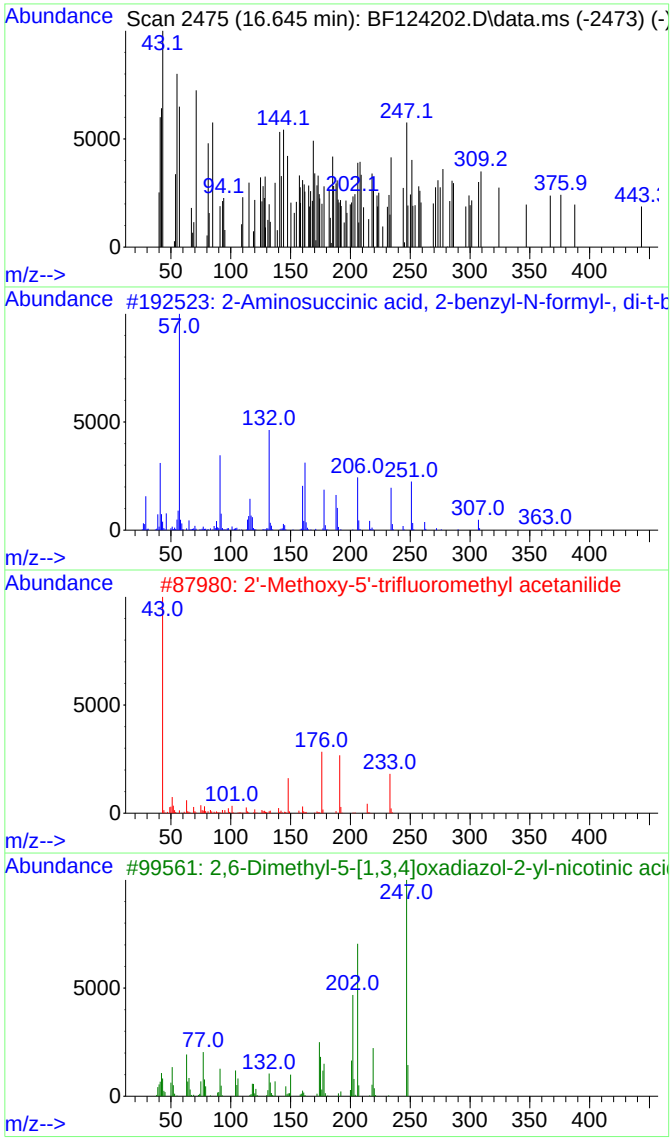
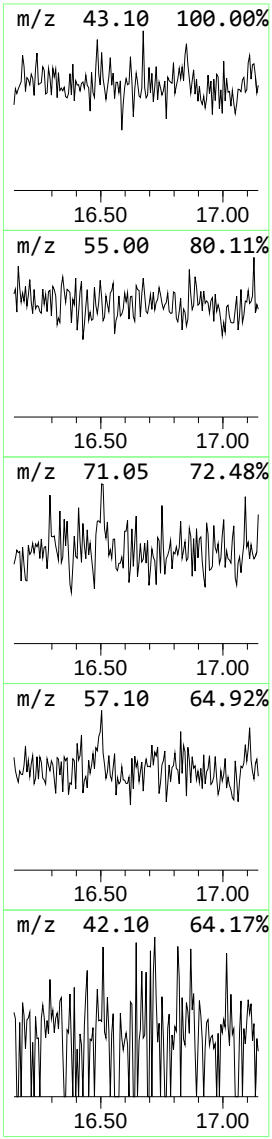
Peak Number 4 unknown16.645 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.645	3.02 ng	30379	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aminosuccinic acid, 2-benzyl-N...	363	C20H29NO5	079435-85-1	12
2	2'-Methoxy-5'-trifluoromethyl ac...	233	C10H10F3NO2	040622-64-8	9
3	2,6-Dimethyl-5-[1,3,4]oxadiazol-...	247	C12H13N3O3	1000301-19-7	9
4	2-Naphthalenecarboxylic acid, 3-...	293	C14H15NO6	089586-22-1	7
5	Perhydro-htx, 1-acetyl-, acetate...	309	C18H31NO3	082260-20-6	7





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentene, 4,4-...	4.440	10.0	ng	100103	1	6.863	200442	20.0
2-Pentanone, 4-...	5.063	7.8	ng	78276	1	6.863	200442	20.0
unknown15.198	15.198	2.5	ng	25169	6	15.527	200877	20.0
unknown16.645	16.645	3.0	ng	30379	6	15.527	200877	20.0