LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124084.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	10	15	22	rVB	115338	133875	31.21%	2.219%
2	2.287	27	34	39	rBV5	7013	10692	2.49%	0.177%
3	3.981	319	322	327	rVB	5615	5150	1.20%	0.085%
4	5.098	509	512	520	rVB	74577	71000	16.55%	1.177%
5	5.504	577	581	589	rBV	245605	221454	51.62%	3.670%
6	5.904	646	649	652	rBV2	7754	6886	1.61%	0.114%
7	6.510	749	752	763	rBV2	220871	223229	52.04%	3.699%
8	6.734	786	790	792	rBV2	3800	4856	1.13%	0.080%
9	6.892	813	817	820	rBV	407739	336957	78.55%	5.584%
10	7.016	835	838	841	rBV2	4936	4980	1.16%	0.083%
11	7.169	860	864	868	rBB	4148	5336	1.24%	0.088%
12	7.445	908	911	916	rVB	162470	145963	34.03%	2.419%
13	7.575	923	933	945	rBV	95272	183440	42.76%	3.040%
14	7.904	983	989	993	rBV	2782	4974	1.16%	0.082%
15	8.104	1020	1023	1027	rVB	11848	9107	2.12%	0.151%
16	8.175	1030	1035	1040	rBV	492483	390707	91.08%	6.475%
17	8.939	1161	1165	1170	rBV	8431	10009	2.33%	0.166%
18	9.245	1214	1217	1226	rBV	291158	263790	61.49%	4.371%
19	9.363	1233	1237	1240	rBV3	10342	12342	2.88%	0.205%
20	9.639	1282	1284	1288	rVB	26471	23456	5.47%	0.389%
21	9.739	1296	1301	1307	rBV4	13727	21348	4.98%	0.354%
22	9.822	1313	1315	1319	rBV	14266	16279	3.79%	0.270%
23	9.933	1330	1334	1343	rBV	447515	428971	100.00%	7.109%
24	10.069	1355	1357	1360	rBV	7183	5821	1.36%	0.096%
25	10.116	1362	1365	1369	rBV	16453	16079	3.75%	0.266%
26	10.216	1377	1382	1386	rBV2	8322	10404	2.43%	0.172%
27	10.298	1386	1396	1402	rBV	295523	333758	77.80%	5.531%
28	10.498	1427	1430	1434	rBV	16598	17131	3.99%	0.284%
29	10.716	1464	1467	1471	rVB	148410	122736	28.61%	2.034%
30	10.775	1474	1477	1481	rBV5	6427	8578	2.00%	0.142%
31	10.833	1485	1487	1492	rVB2	4858	7000	1.63%	0.116%
32	11.157	1538	1542	1545	rBV	95694	80246	18.71%	1.330%
33	11.280	1558	1563	1566	rBV4	7677	9815	2.29%	0.163%
34	11.333	1571	1572	1576	rVB2	6289	5533	1.29%	0.092%
35	11.416	1583	1586	1590	rBV	390115	358488	83.57%	5.941%
36	11.551	1606	1609	1611	rBV4	4428	6335	1.48%	0.105%

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.704	1631	1635	1636	rBV3	4449	5228	1.22%	0.087%
38	11.745	1639	1642	1645	rVB4	9684	11723	2.73%	0.194%
39	11.780	1645	1648	1650	rBV4	5655	8316	1.94%	0.138%
40	11.886	1664	1666	1669	rBV3	4468	5958	1.39%	0.099%
41	11.939	1672	1675	1681	rVV5	33207	43326	10.10%	0.718%
42	12.004	1683	1686	1690	rVV3	44276	45036	10.50%	0.746%
43	12.069	1694	1697	1700	rVV	30777	22200	5.18%	0.368%
44	12.139	1706	1709	1710	rBV3	14720	10932	2.55%	0.181%
45	12.174	1713	1715	1717	rBV3	4536	5143	1.20%	0.085%
46	12.233	1723	1725	1726	rBV2	8450	5636	1.31%	0.093%
47	12.321	1733	1740	1742	rBV8	5496	10302	2.40%	0.171%
48	12.339	1742	1743	1746	rBV3	4881	4806	1.12%	0.080%
49	12.374	1746	1749	1752	rBV4	7109	9130	2.13%	0.151%
50	12.421	1756	1757	1758	rBV	9990	5147	1.20%	0.085%
51	12.439	1758	1760	1763	rVB3	16091	12614	2.94%	0.209%
52	12.469	1763	1765	1767	rVB3	6656	5782	1.35%	0.096%
53	12.498	1767	1770	1771	rBV2	10576	11620	2.71%	0.193%
54	12.651	1791	1796	1803	rBV10	19608	43242	10.08%	0.717%
55	12.704	1803	1805	1806	rBV	6536	5891	1.37%	0.098%
56	12.733	1808	1810	1813	rVB4	13595	13628	3.18%	0.226%
57	12.780	1815	1818	1820	rBV3	19843	18289	4.26%	0.303%
58	13.004	1852	1856	1859	rVB	246533	206223	48.07%	3.417%
59	13.121	1872	1876	1877	rBV4	9721	10448	2.44%	0.173%
60	13.192	1886	1888	1891	rBV4	10731	7789	1.82%	0.129%
61	13.304	1904	1907	1910	rBV	51159	39564	9.22%	0.656%
62	13.357	1914	1916	1919	rVB2	31742	21935	5.11%	0.364%
63	13.492	1935	1939	1943	rBV3	50261	56458	13.16%	0.936%
64	13.768	1984	1986	1989	rBV3	13834	13731	3.20%	0.228%
65	13.904	2007	2009	2012	rBV4	13976	12824	2.99%	0.213%
66	13.945	2012	2016	2021	rVB7	53638	70343	16.40%	1.166%
67	13.992	2022	2024	2025	rBV2	17385	14621	3.41%	0.242%
68	14.039	2029	2032	2033	rVV2	80995	62674	14.61%	1.039%
69	14.063	2033	2036	2039	rVB	332926	288680	67.30%	4.784%
70	14.292	2072	2075	2078	rBV2	70192	98222	22.90%	1.628%
71	14.327	2079	2081	2086	rVB2	57698	49861	11.62%	0.826%
72	14.374	2086	2089	2095	rVB	74658	83501	19.47%	1.384%
73	14.439	2096	2100	2104	rBV2	263387	422179	98.42%	6.996%
74	14.510	2109	2112	2118	rBV	88746	111097	25.90%	1.841%
75	14.580	2122	2124	2125	rBV	62222	55185	12.86%	0.915%
76	14.698	2140	2144	2150	rVB2	107612	130562	30.44%	2.164%

LSC Area Percent Report

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Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	14.833	2164	2167	2171	rVB	66771	65791	15.34%	1.090%
78	14.898	2175	2178	2183	rVB2	59900	74377	17.34%	1.233%
79	15.557	2286	2290	2299	rVB2	196053	317635	74.05%	5.264%

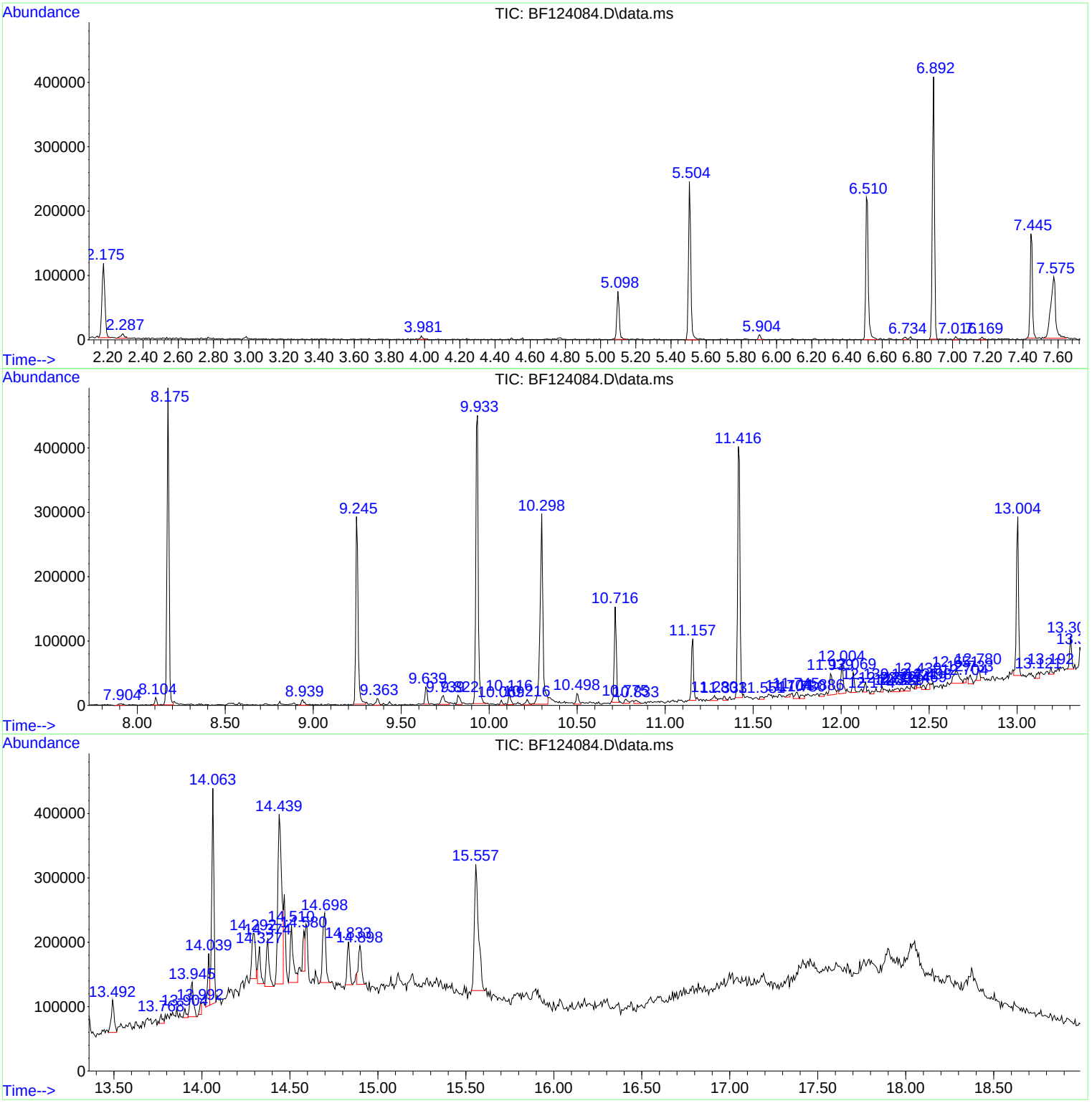
Sum of corrected areas: 6034374

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

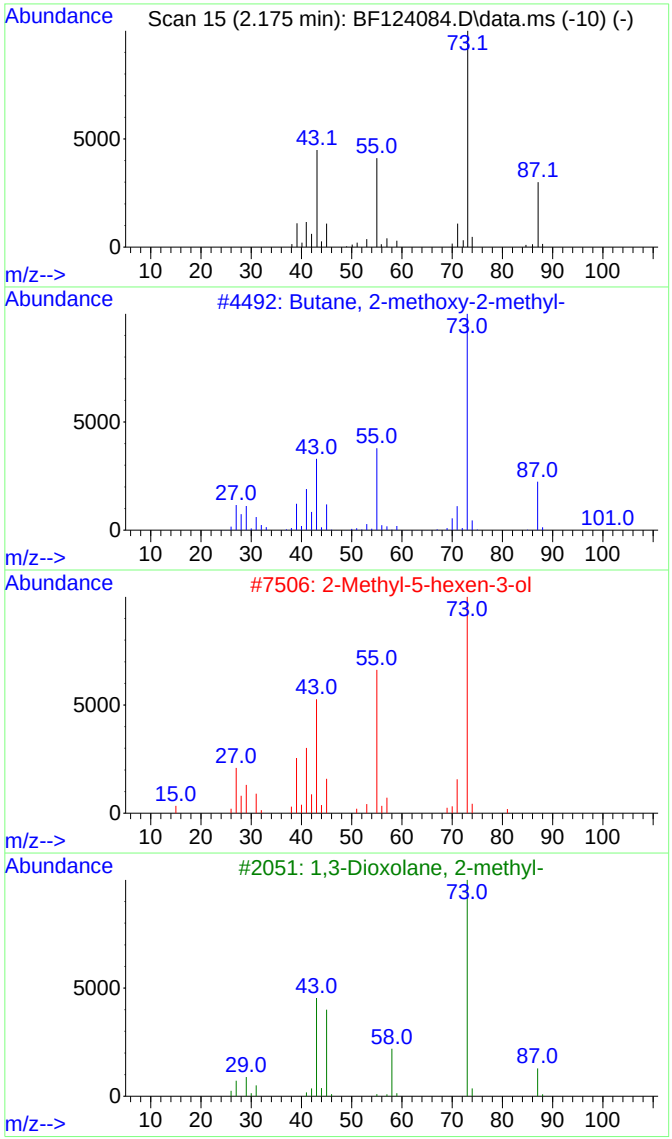
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

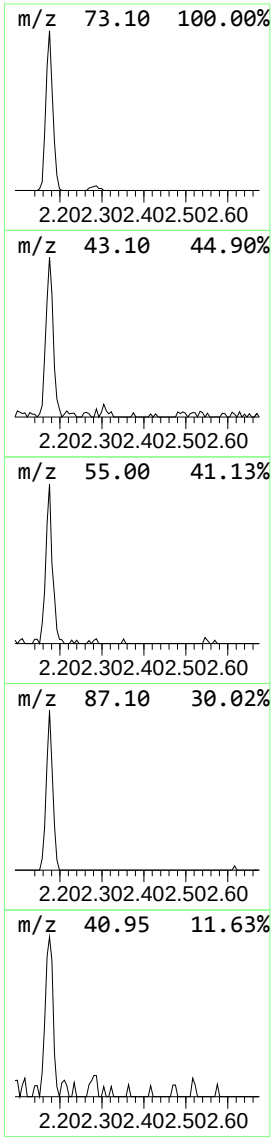
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	7.95 ng	133875	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
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Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

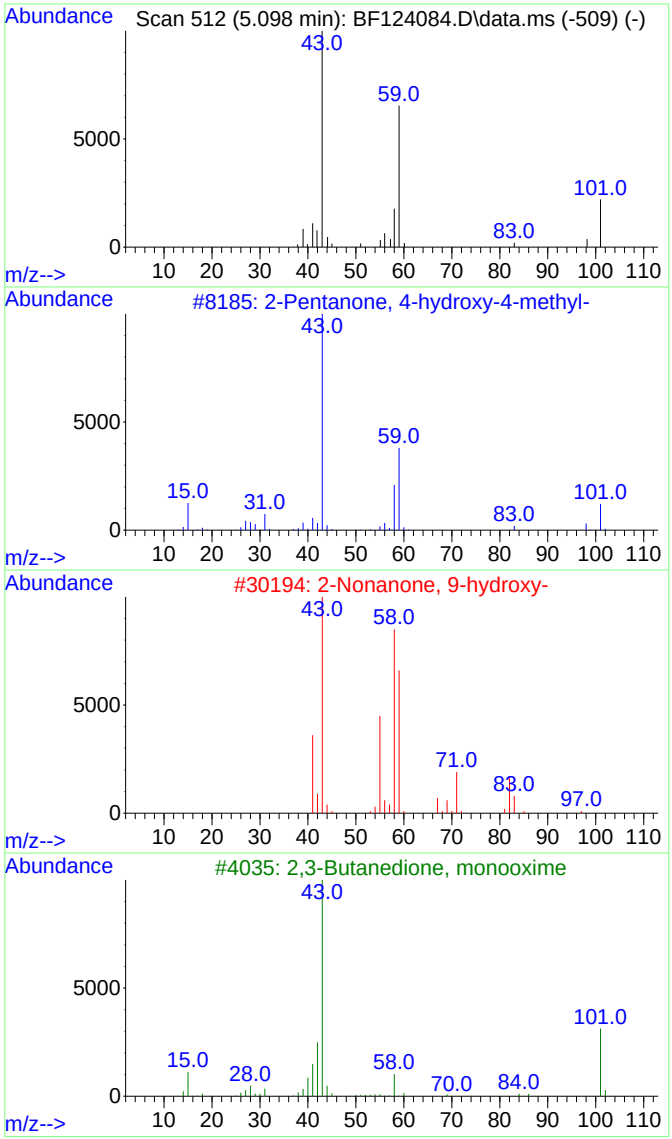
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

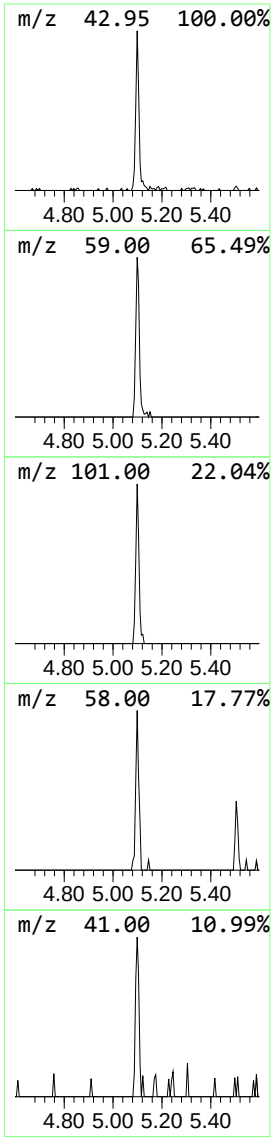
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	4.21 ng	71000	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

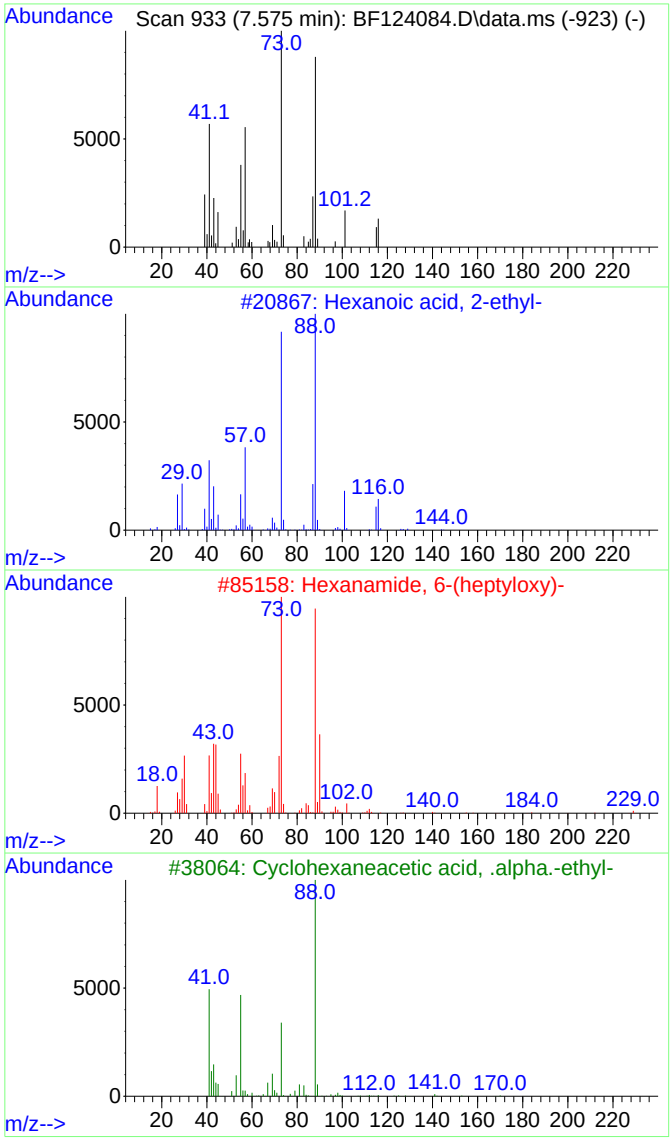
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

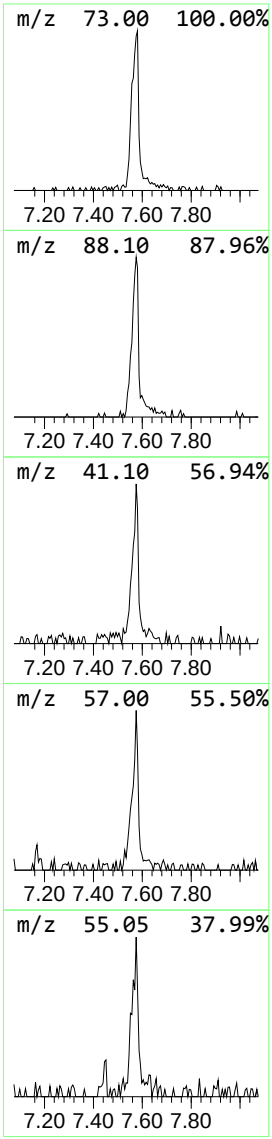
****

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	9.39 ng	183440	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	50
3	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	40
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38
5	Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	38





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

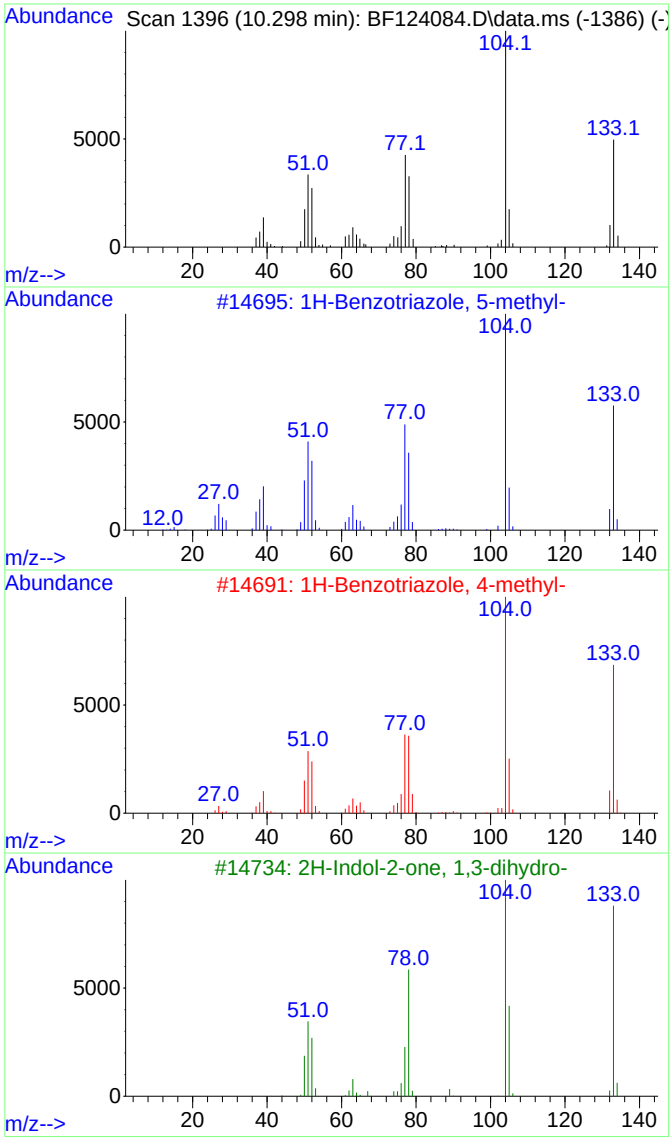
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

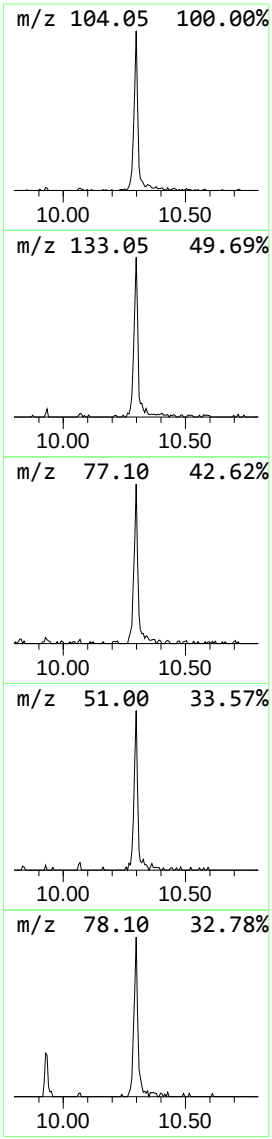
****

Peak Number 4 1H-Benzotriazole, 5-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.298	15.56 ng	333758	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	98
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	97
3	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	68
4	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	64
5	2-Pyridinecarbonitrile	104	C6H4N2	000100-70-9	50





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Misc :
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Instrument : BNA_F
ClientSampleId : 115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

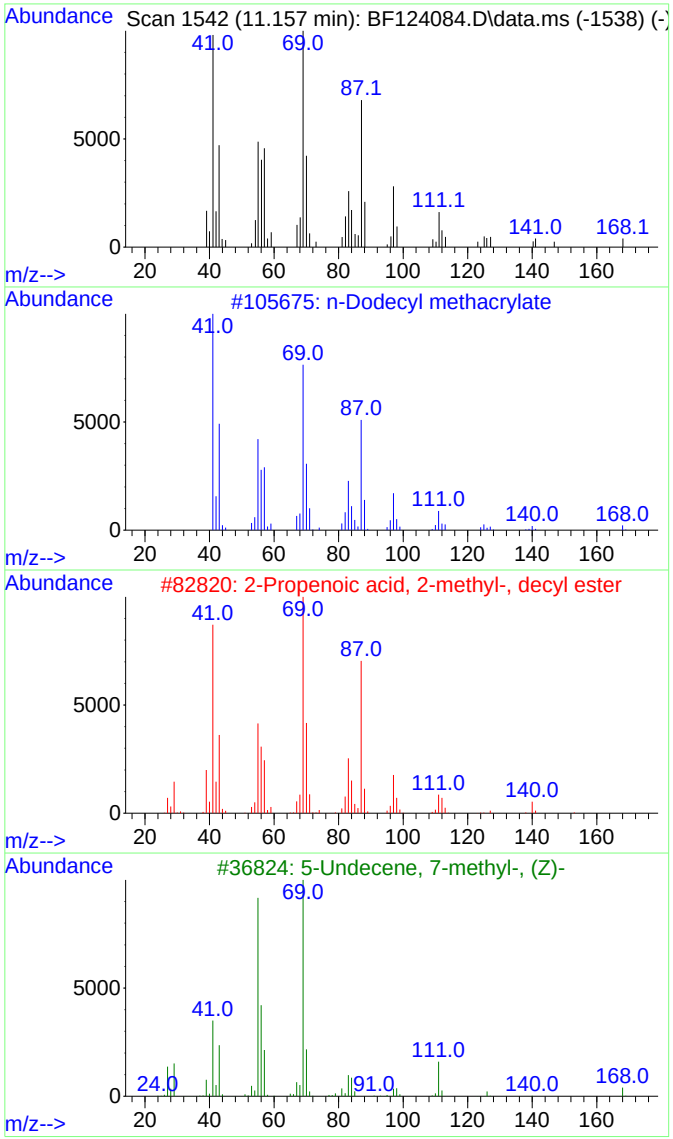
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

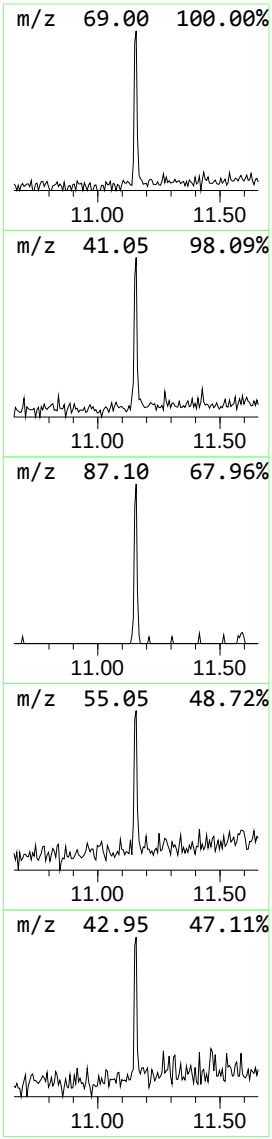
****

Peak Number 5 n-Dodecyl methacrylate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.157	4.48 ng	80246	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	87
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	87
3	5-Undecene, 7-methyl-, (Z)-	168	C12H24	074630-62-9	47
4	Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	46
5	Cyclohexanone, 3-methyl-	112	C7H12O	000591-24-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

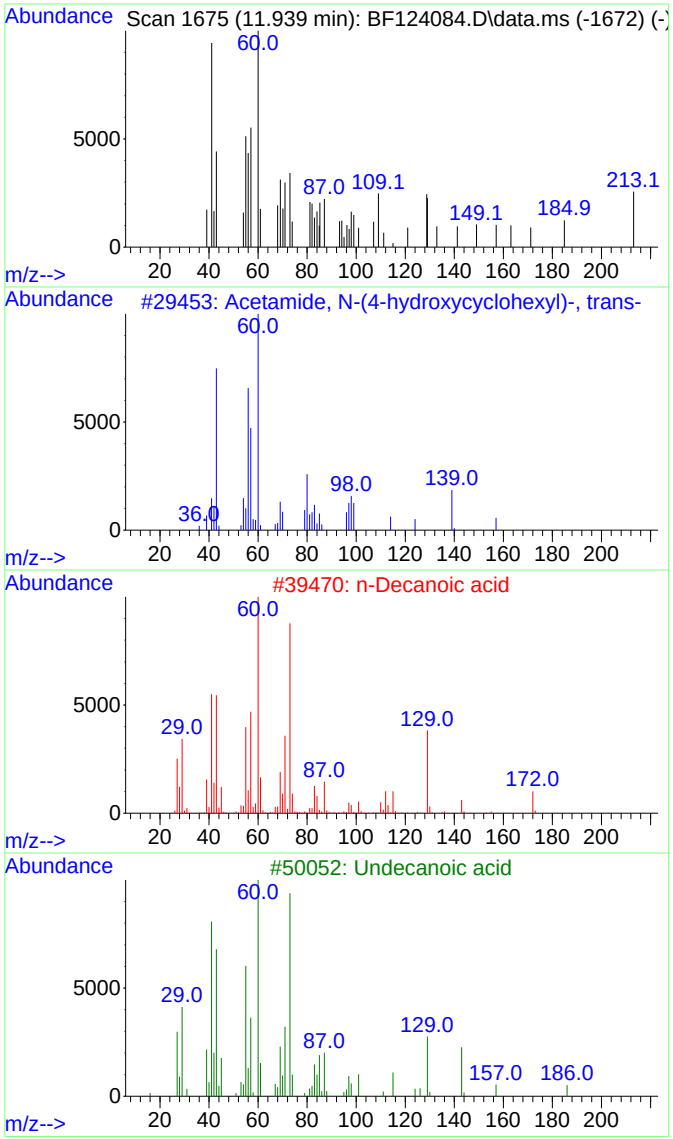
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

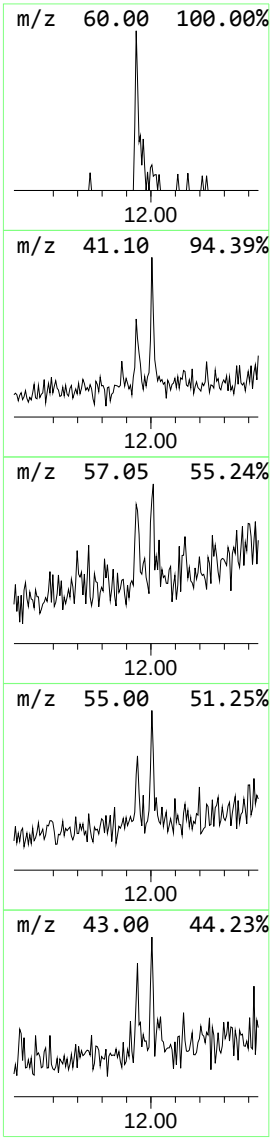
****

Peak Number 6 unknown11.939 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.42 ng	43326	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(4-hydroxycyclohexy...	157	C8H15NO2	027489-60-7	35
2	n-Decanoic acid	172	C10H20O2	000334-48-5	35
3	Undecanoic acid	186	C11H22O2	000112-37-8	35
4	Dodecanoic acid	200	C12H24O2	000143-07-7	32
5	Heptanoic acid	130	C7H14O2	000111-14-8	27





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Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

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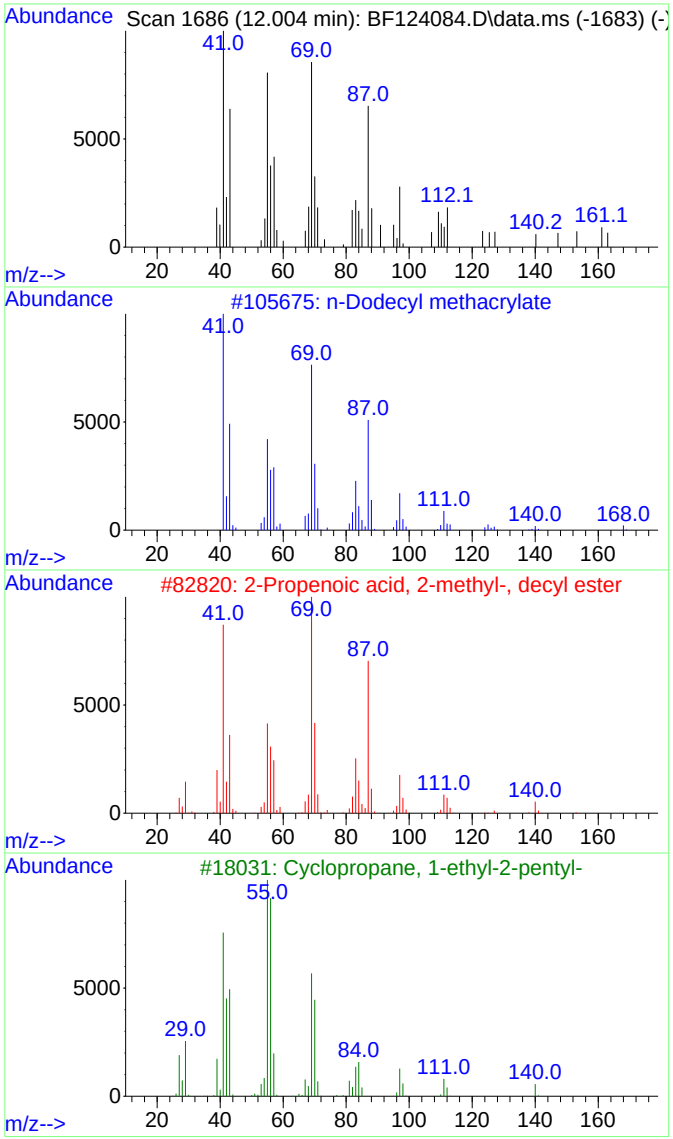
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

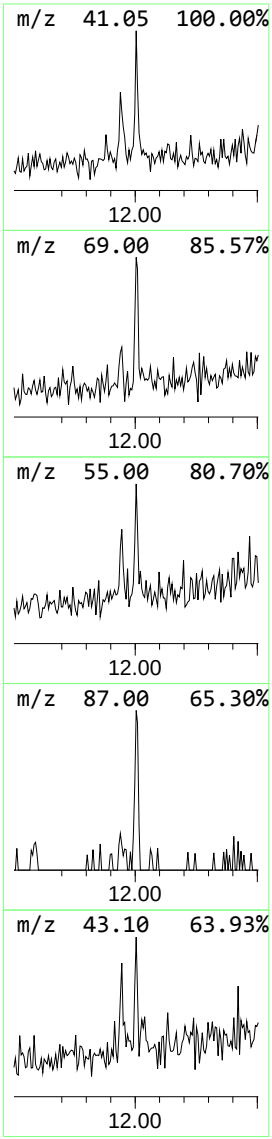
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Propenoic acid, 2-methyl-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.51 ng	45036	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	53
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	53
3	Cyclopropane, 1-ethyl-2-pentyl-	140	C10H20	062238-08-8	38
4	3-Heptene, 4-methyl-	112	C8H16	004485-16-9	35
5	3-Octene, 4-ethyl-	140	C10H20	053966-51-1	35





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Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

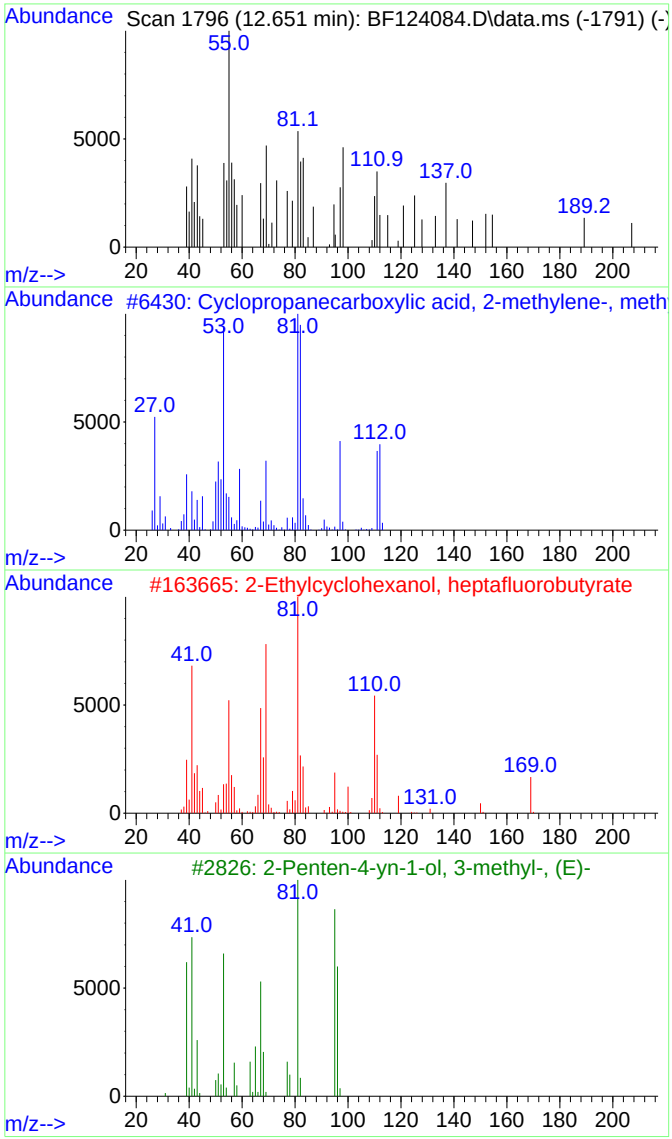
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

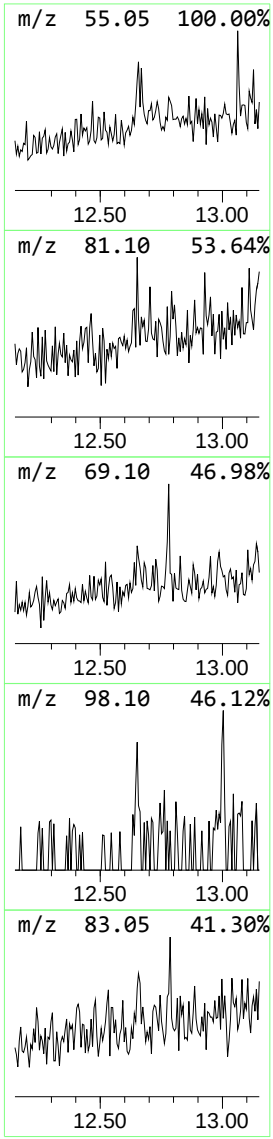
****

Peak Number 8 unknown12.651 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.41 ng	43242	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 2-m...	112	C6H8O2	088787-23-9	43
2	2-Ethylcyclohexanol, heptafluoro...	324	C12H15F7O2	959079-92-6	37
3	2-Penten-4-yn-1-ol, 3-methyl-, (E)-	96	C6H8O	006153-06-6	35
4	Metronidazole	171	C6H9N3O3	000443-48-1	35
5	10-Undecenal	168	C11H20O	000112-45-8	16





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Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

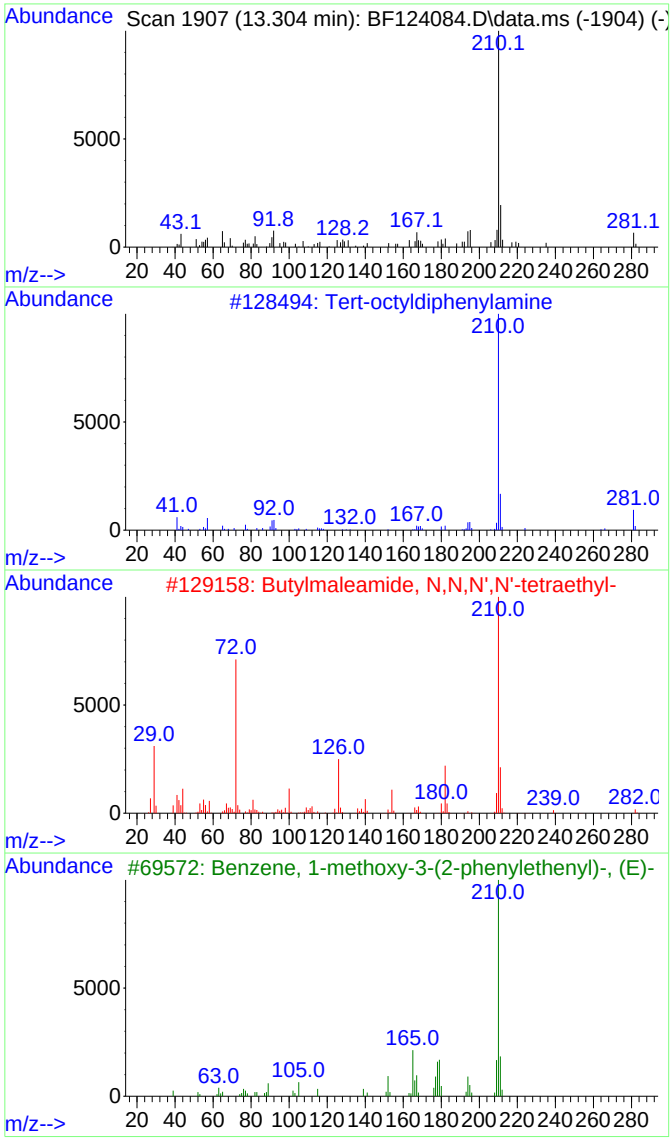
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

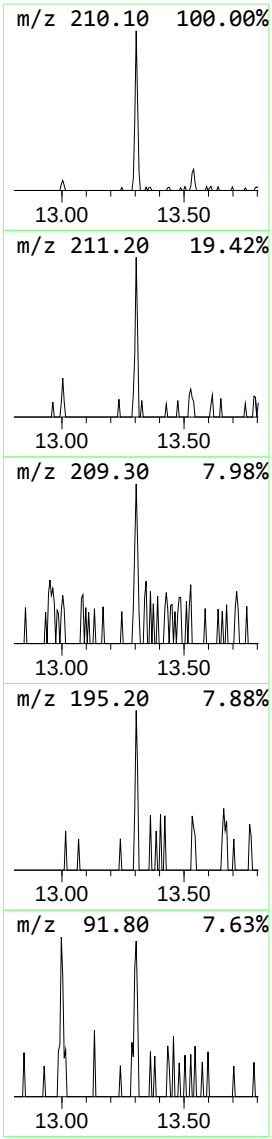
****

Peak Number 9 Tert-octyldiphenylamine Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.304	2.74 ng	39564	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tert-octyldiphenylamine	281	C20H27N	1000370-31-3	90
2	Butylmaleamide, N,N,N',N'-tetrae...	282	C16H30N2O2	095503-13-2	80
3	Benzene, 1-methoxy-3-(2-phenylet...	210	C15H14O	014064-41-6	80
4	9H-Carbazol-3-amine, 9-ethyl-	210	C14H14N2	000132-32-1	80
5	1,2-Phenanthrenediamine, 9,10-di...	210	C14H14N2	018264-92-1	78





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Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

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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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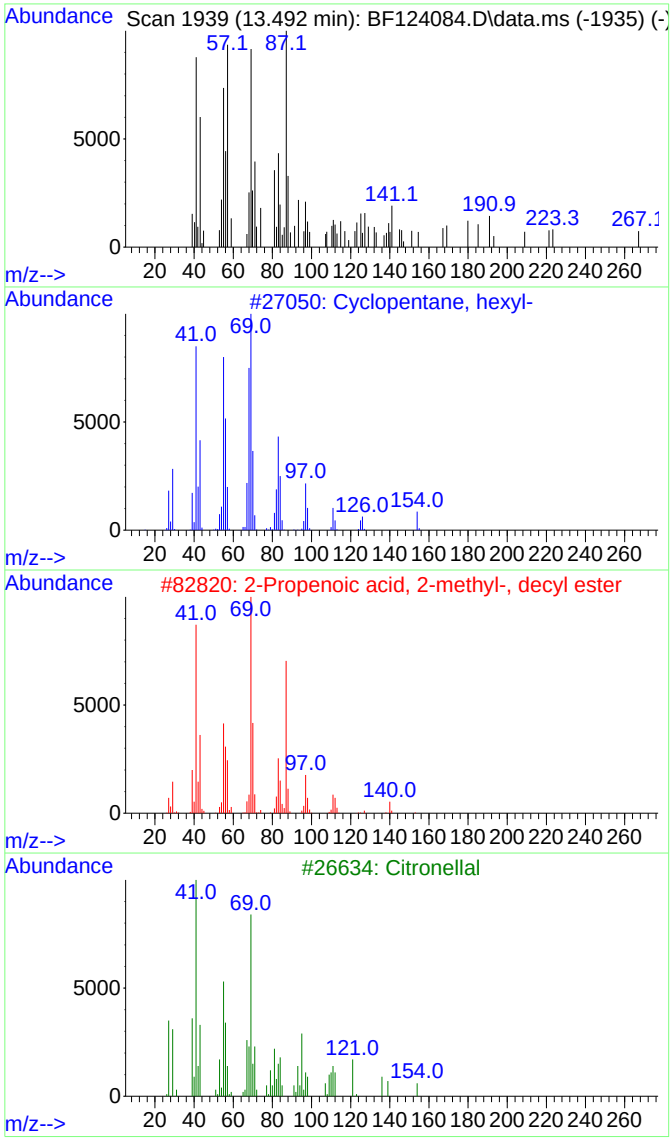
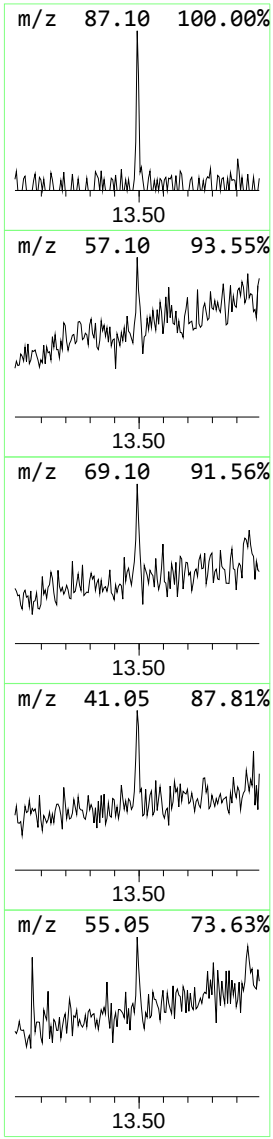
Peak Number 10 Cyclopentane, hexyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	3.91 ng	56458	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, hexyl-	154	C11H22	004457-00-5	70
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	46
3	Citronellal	154	C10H18O	000106-23-0	46
4	Cyclopentane, propyl-	112	C8H16	002040-96-2	30
5	Nonane, 2-methyl-3-methylene-	154	C11H22	055499-08-6	30





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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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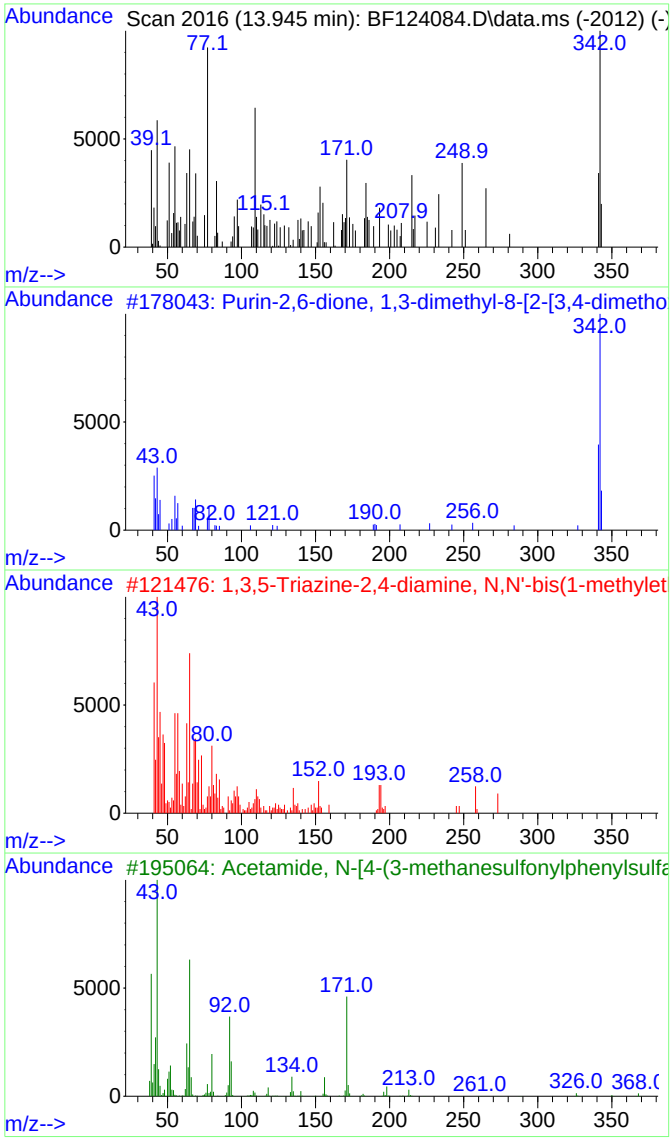
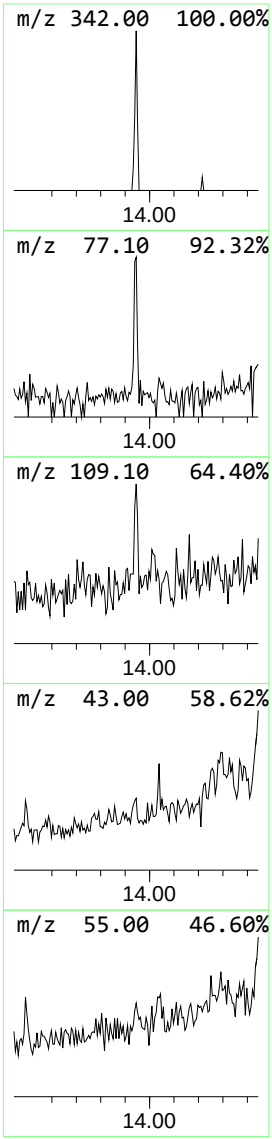
Peak Number 11 unknown13.945 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	4.87 ng	70343	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Purin-2,6-dione, 1,3-dimethyl-8-...	342	C17H18N4O4	1000127-57-8	15
2	1,3,5-Triazine-2,4-diamine, N,N'...	273	C10H19N5O2S	055723-98-3	12
3	Acetamide, N-[4-(3-methanesulfon...	368	C15H16N2O5S2	1000311-21-2	12
4	Tetradehydroabietic acid, 7-meth...	342	C22H30O3	197444-13-6	11
5	Phenyl chloroformate	156	C7H5ClO2	001885-14-9	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

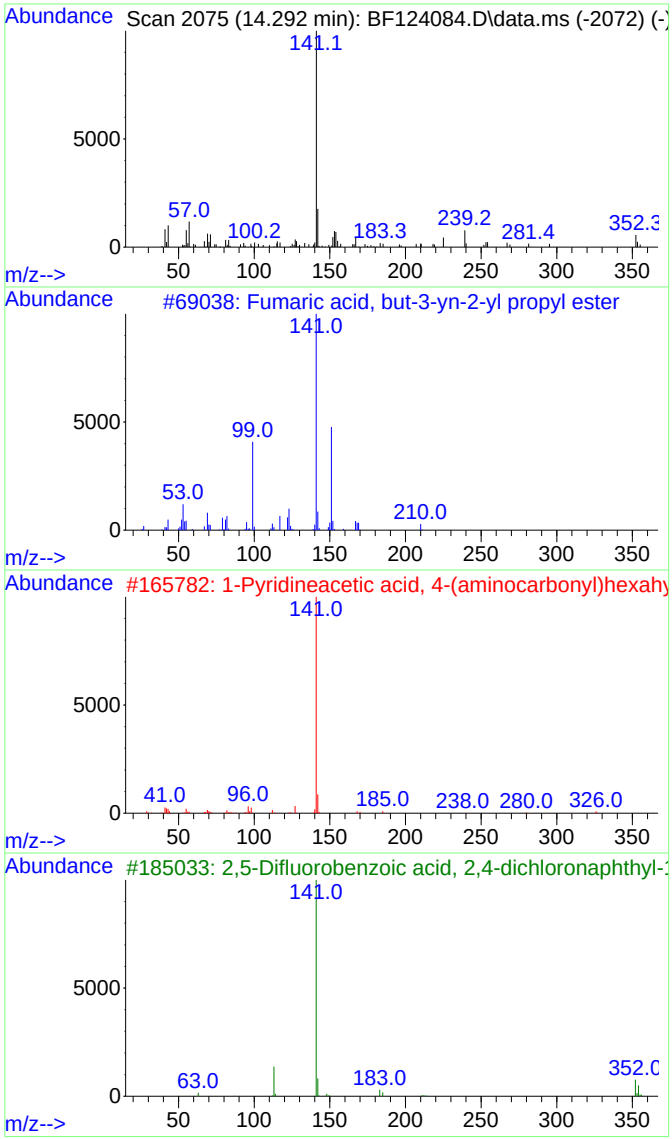
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

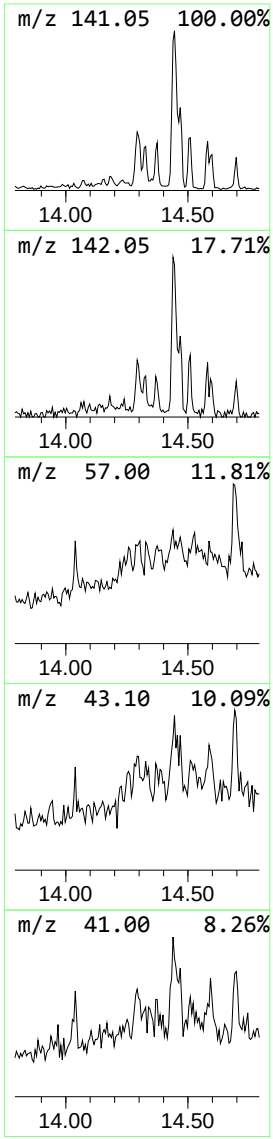
****

Peak Number 12 Fumaric acid, but-3-yn-2-yl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.292	6.80 ng	98222	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, but-3-yn-2-yl prop...	210	C11H14O4	1000345-27-7	59
2	1-Pyridineacetic acid, 4-(aminoc...	326	C18H34N2O3	1000319-12-3	59
3	2,5-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-56-9	56
4	2,4-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-58-5	50
5	3,4-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-64-4	50





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Sample : M2518-01 5X
Misc :
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Instrument : BNA_F
ClientSampleId : 115

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

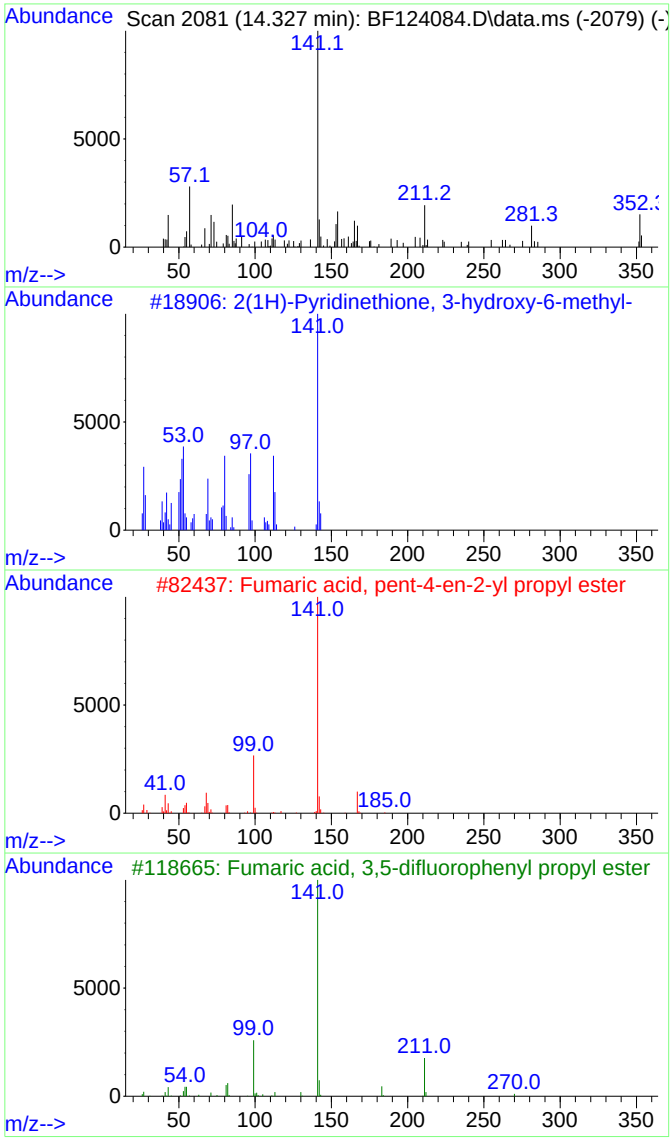
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

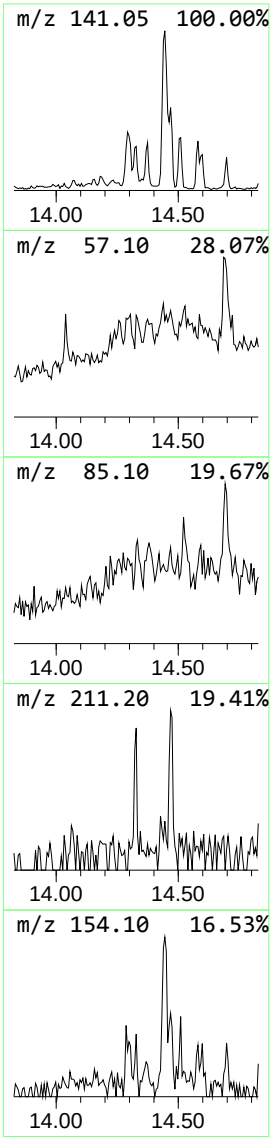
****

Peak Number 13 unknown14.327 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	3.45 ng	49861	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyridinethione, 3-hydroxy-...	141	C6H7NOS	022989-67-9	38
2	Fumaric acid, pent-4-en-2-yl pro...	226	C12H18O4	1000348-92-1	38
3	Fumaric acid, 3,5-difluorophenyl...	270	C13H12F2O4	1000339-36-8	37
4	Thiazole, 2-ethyl-4,5-dimethyl-	141	C7H11NS	000873-64-3	37
5	Fumaric acid, phenyl propyl ester	234	C13H14O4	1000339-36-1	35





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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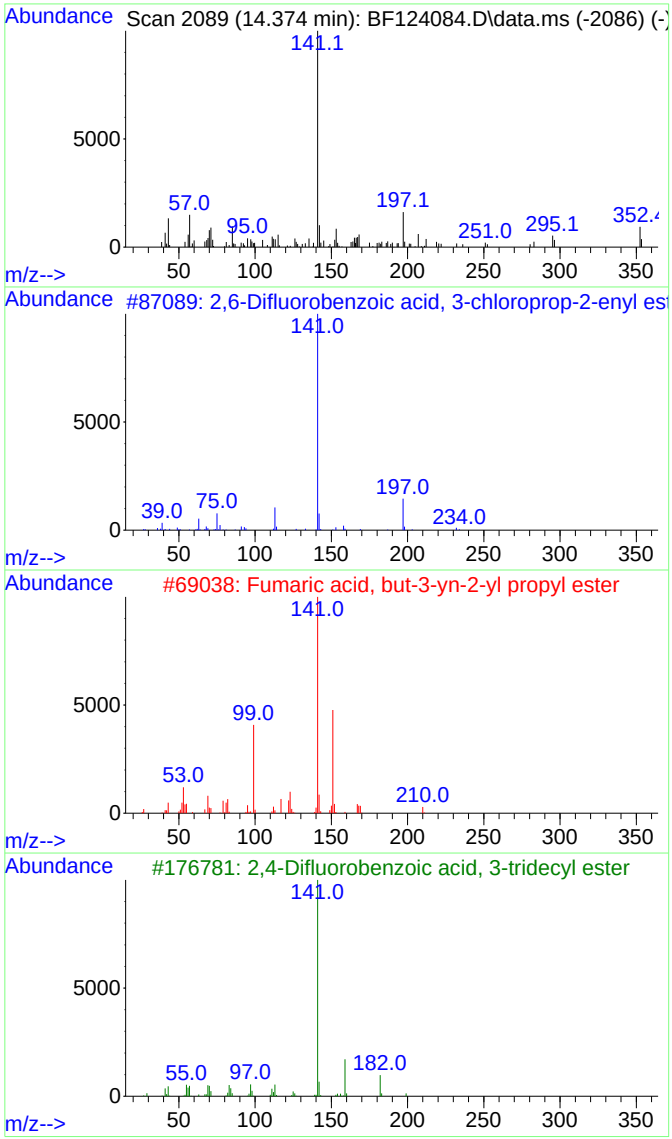
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

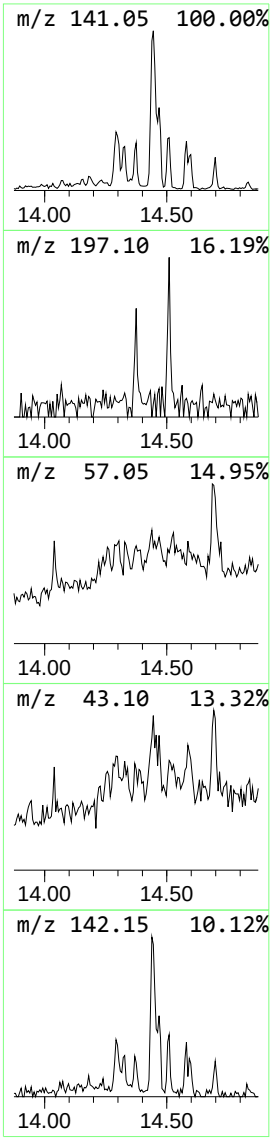
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2,6-Difluorobenzoic acid, 3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.374	5.79 ng	83501	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Difluorobenzoic acid, 3-chlo...	232	C10H7ClF2O2	1000292-59-0	53
2	Fumaric acid, but-3-yn-2-yl prop...	210	C11H14O4	1000345-27-7	50
3	2,4-Difluorobenzoic acid, 3-trid...	340	C20H30F2O2	1000338-56-8	50
4	2,4-Difluorobenzoic acid, 4-trid...	340	C20H30F2O2	1000338-56-9	50
5	2,6-Difluorobenzoic acid, pent-2...	222	C12H8F2O2	1000292-58-3	50





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Sample : M2518-01 5X
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
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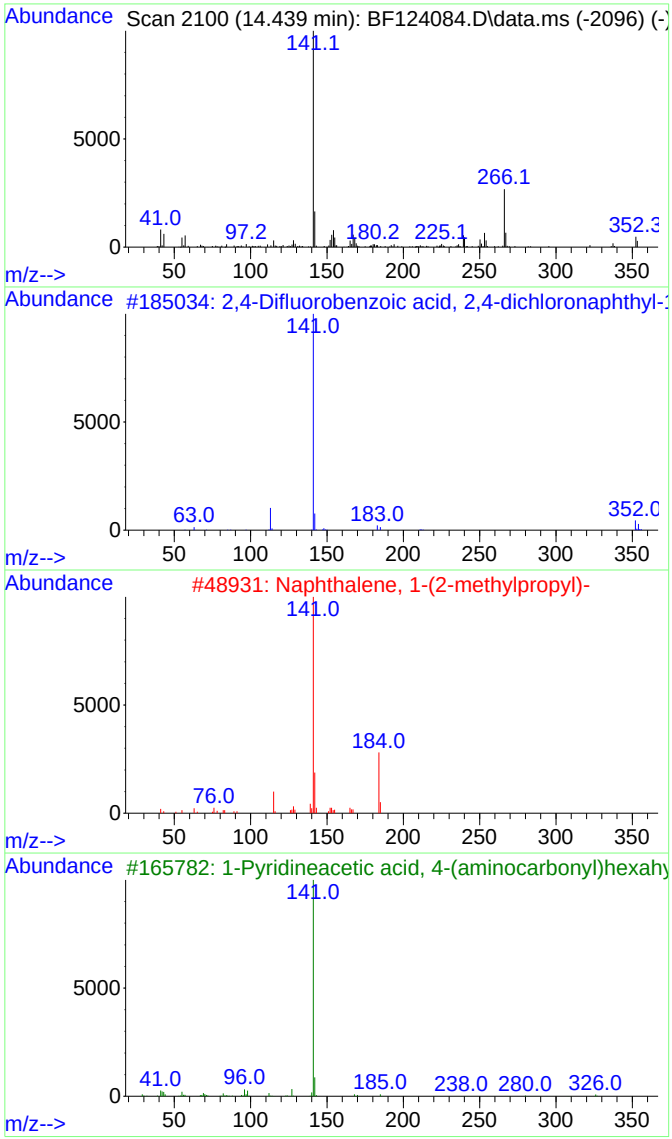
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

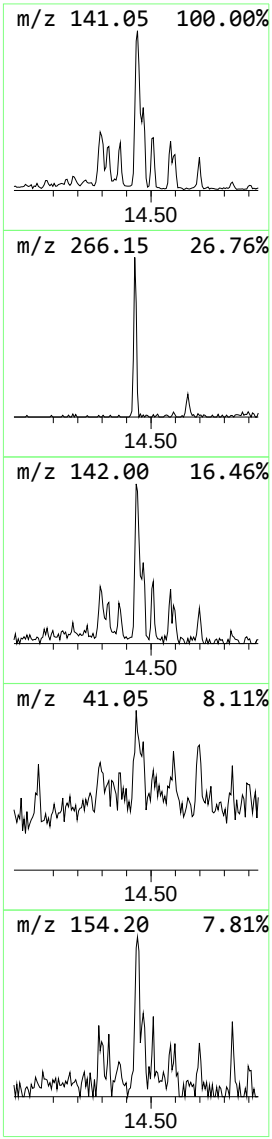
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 2,4-Difluorobenzoic acid, 2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	29.25 ng	422179	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-58-5	53
2	Naphthalene, 1-(2-methylpropyl)-	184	C14H16	016727-91-6	50
3	1-Pyridineacetic acid, 4-(aminoc...	326	C18H34N2O3	1000319-12-3	50
4	2,5-Pyrrolidinedione, 1,3-diethy...	169	C9H15NO2	054410-85-4	38
5	2,6-Difluorobenzoic acid, 2,4,6-...	336	C13H5Cl3F2O2	1000325-74-2	38





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ClientSampleId : 115

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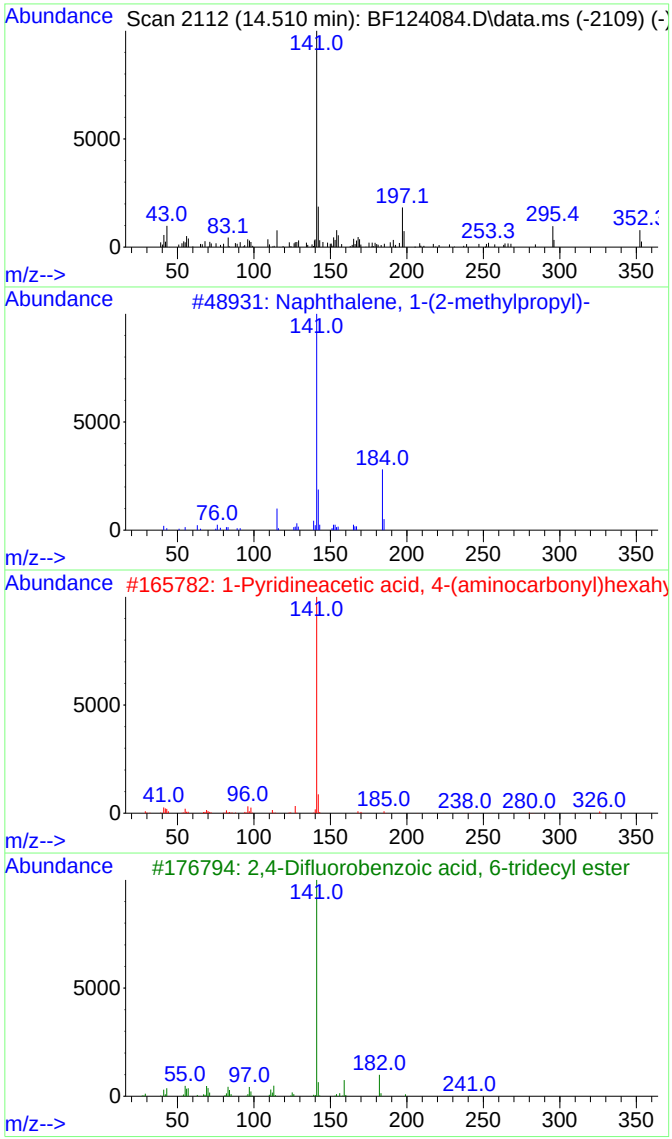
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

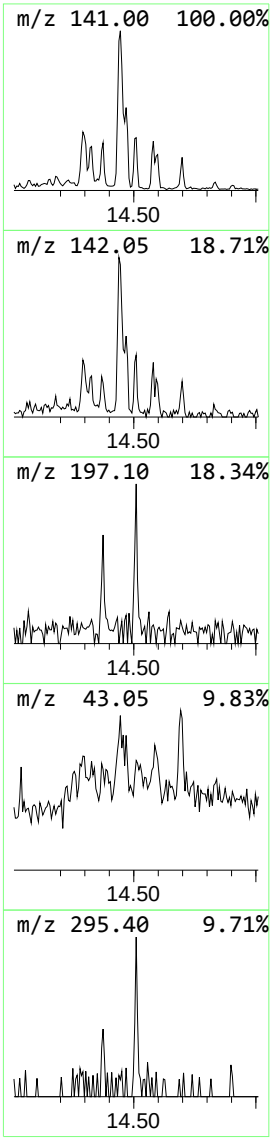
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Naphthalene, 1-(2-methylpro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	7.70 ng	111097	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-(2-methylpropyl)-	184	C14H16	016727-91-6	53
2	1-Pyridineacetic acid, 4-(aminoc...	326	C18H34N2O3	1000319-12-3	50
3	2,4-Difluorobenzoic acid, 6-trid...	340	C20H30F2O2	1000338-57-1	50
4	Naphthalene, 1-propyl-	170	C13H14	002765-18-6	42
5	1-But-3-enylnaphthalene	182	C14H14	002489-88-5	42





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
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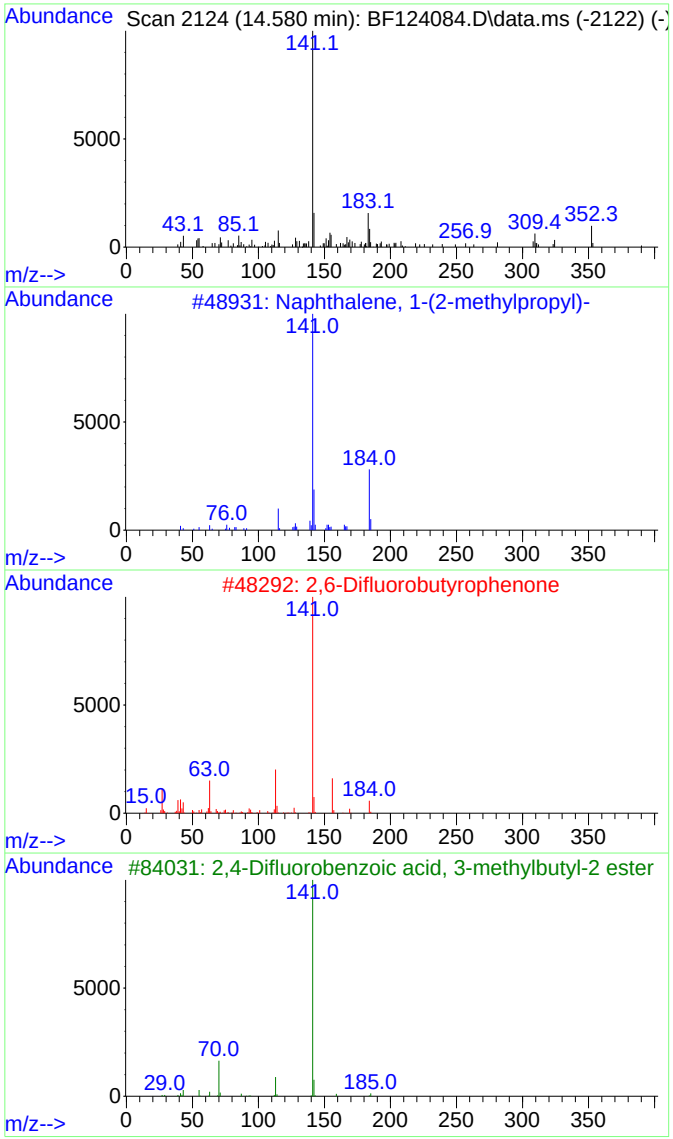
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

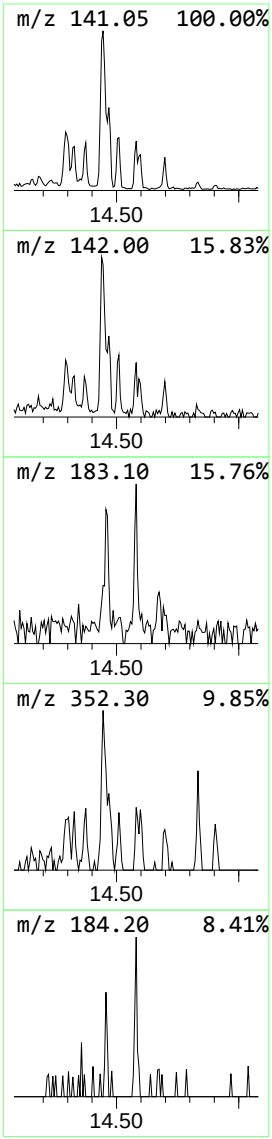
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 2,6-Difluorobutyrophenone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	3.82 ng	55185	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-(2-methylpropyl)-	184	C14H16	016727-91-6	53
2	2,6-Difluorobutyrophenone	184	C10H10F2O	095727-77-8	53
3	2,4-Difluorobenzoic acid, 3-meth...	228	C12H14F2O2	1000360-55-3	53
4	2,5-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-56-9	50
5	2-Chloro-2',4'-difluoroacetophenone	190	C8H5ClF2O	051336-94-8	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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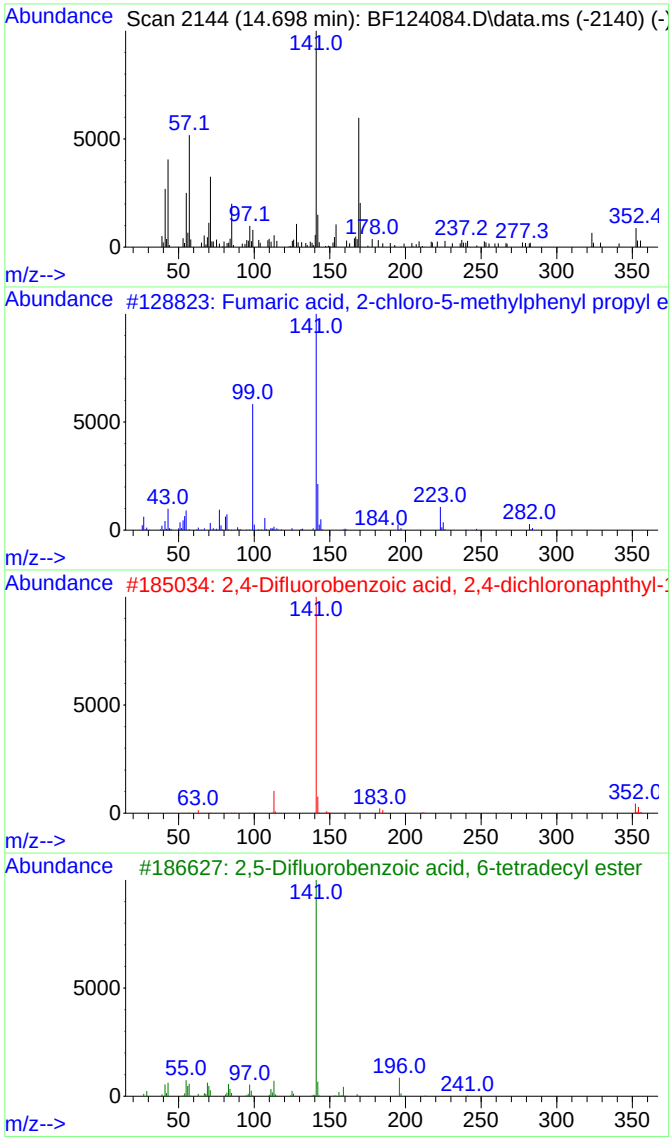
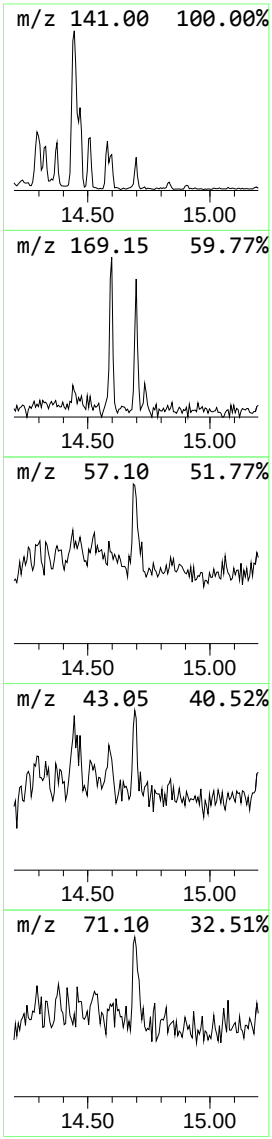
Peak Number 18 unknown14.698 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	9.05 ng	130562	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloro-5-methylp...	282	C14H15ClO4	1000348-25-5	35
2	2,4-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-58-5	35
3	2,5-Difluorobenzoic acid, 6-tetr...	354	C21H32F2O2	1000338-48-2	27
4	Nonanoic acid, 4-nitrophenyl ester	279	C15H21NO4	1000358-02-8	27
5	2,4-Difluorobenzoic acid, 4-trid...	340	C20H30F2O2	1000338-56-9	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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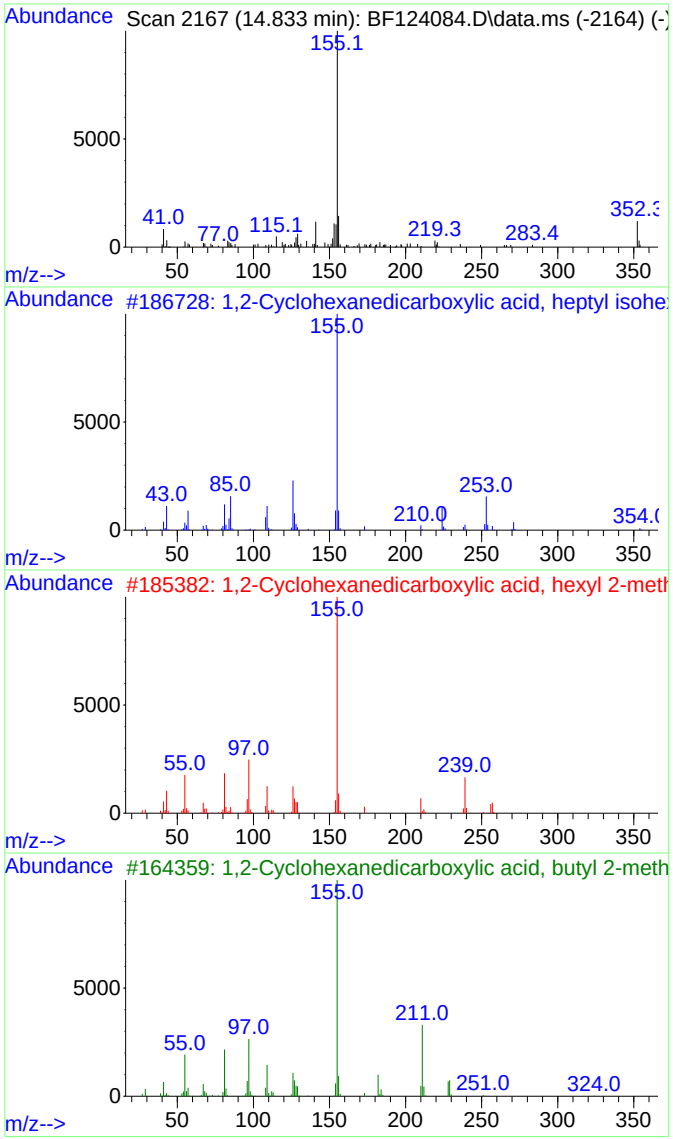
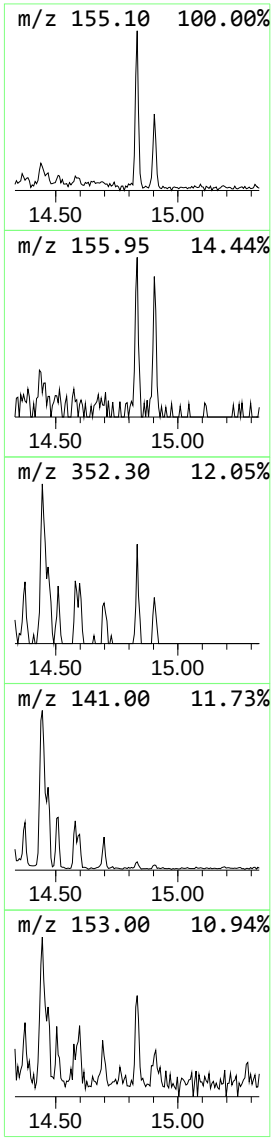
Peak Number 19 1,2-Cyclohexanedicarboxylic... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	4.14 ng	65791	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-53-6	53
2	1,2-Cyclohexanedicarboxylic acid...	352	C21H36O4	1000339-88-0	53
3	1,2-Cyclohexanedicarboxylic acid...	324	C19H32O4	1000339-87-7	53
4	1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-45-4	53
5	1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-47-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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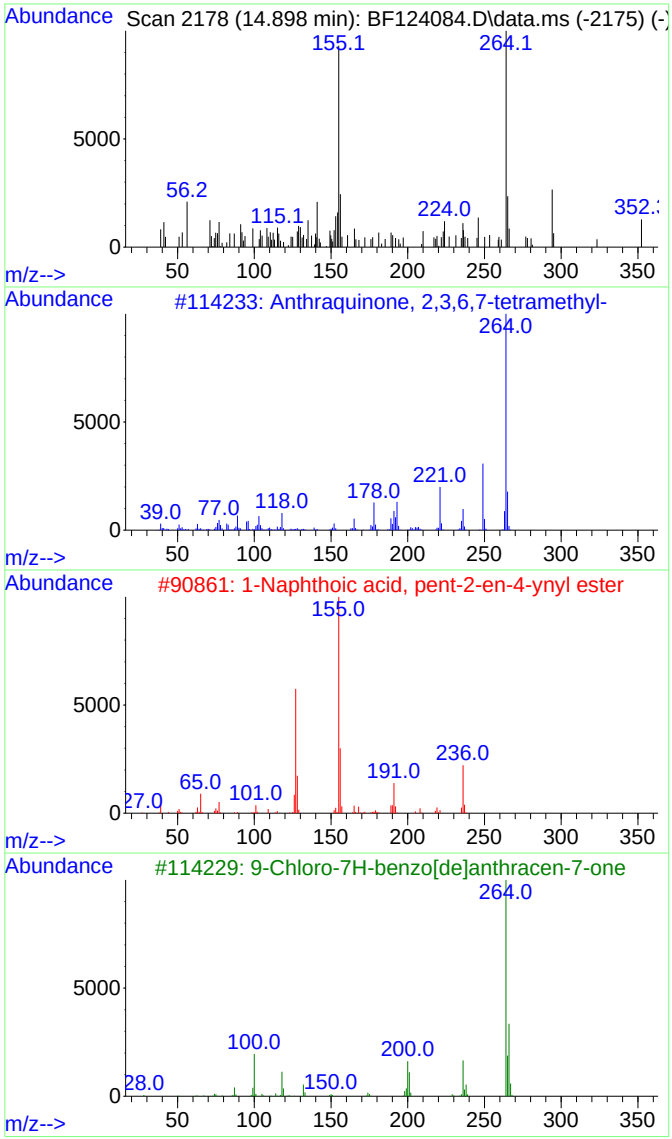
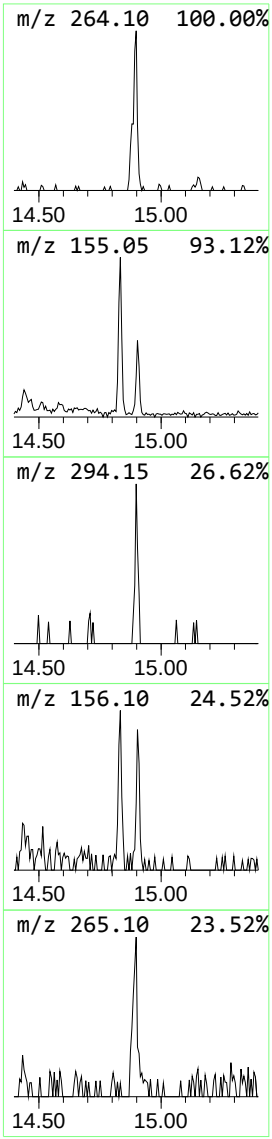
Peak Number 20 unknown14.898 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	4.68 ng	74377	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthraquinone, 2,3,6,7-tetramethyl-	264	C18H16O2	015247-68-4	38
2	1-Naphthoic acid, pent-2-en-4-yn...	236	C16H12O2	1000308-82-0	30
3	9-Chloro-7H-benzo[de]anthracen-7...	264	C17H9ClO	024092-47-5	27
4	Chromeno(4,3-c)chromene-5,11-dione	264	C16H8O4	013225-81-5	25
5	1-(4-Methoxyphenyl)piperazine, 4...	264	C14H24N2OSi	1000373-99-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124084.D
Acq On : 27 May 2021 2:06
Operator : JU/CG
Sample : M2518-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 115

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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
Butane, 2-metho...	2.175	8.0	ng	133875	1	6.892	336957	20.0
2-Pentanone, 4-...	5.098	4.2	ng	71000	1	6.892	336957	20.0
Hexanoic acid, ...	7.575	9.4	ng	183440	2	8.175	390707	20.0
1H-Benzotriazol...	10.298	15.6	ng	333758	3	9.933	428971	20.0
n-Dodecyl metha...	11.157	4.5	ng	80246	4	11.416	358488	20.0
unknown11.939	11.939	2.4	ng	43326	4	11.416	358488	20.0
2-Propenoic aci...	12.004	2.5	ng	45036	4	11.416	358488	20.0
unknown12.651	12.651	2.4	ng	43242	4	11.416	358488	20.0
Tert-octyldiphe...	13.304	2.7	ng	39564	5	14.063	288680	20.0
Cyclopentane, h...	13.492	3.9	ng	56458	5	14.063	288680	20.0
unknown13.945	13.945	4.9	ng	70343	5	14.063	288680	20.0
Fumaric acid, b...	14.292	6.8	ng	98222	5	14.063	288680	20.0
unknown14.327	14.327	3.5	ng	49861	5	14.063	288680	20.0
2,6-Difluoroben...	14.374	5.8	ng	83501	5	14.063	288680	20.0
2,4-Difluoroben...	14.439	29.3	ng	422179	5	14.063	288680	20.0
Naphthalene, 1-...	14.510	7.7	ng	111097	5	14.063	288680	20.0
2,6-Difluorobut...	14.580	3.8	ng	55185	5	14.063	288680	20.0
unknown14.698	14.698	9.1	ng	130562	5	14.063	288680	20.0
1,2-Cyclohexane...	14.833	4.1	ng	65791	6	15.557	317635	20.0
unknown14.898	14.898	4.7	ng	74377	6	15.557	317635	20.0