LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 282

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-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124883.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	573	577	580	rBV	90102	77000	66.79%	7.330%
2	6.498	746	750	753	rBV	91577	84461	73.26%	8.040%
3	6.869	810	813	816	rBB	58057	43717	37.92%	4.162%
4	7.433	905	909	912	rBB	72456	58106	50.40%	5.532%
5	8.051	1012	1014	1018	rBB	2890	2780	2.41%	0.265%
6	8.151	1028	1031	1035	rBV	70495	62223	53.97%	5.923%
7	9.227	1210	1214	1217	rBV	156597	115292	100.00%	10.976%
8	9.910	1327	1330	1337	rBB	91015	73600	63.84%	7.007%
9	10.310	1395	1398	1400	rBB	2743	2083	1.81%	0.198%
10	10.698	1461	1464	1468	rBV	75821	63220	54.83%	6.018%
11	10.769	1473	1476	1480	rBV3	1264	1811	1.57%	0.172%
12	10.810	1480	1483	1487	rBV2	3950	6306	5.47%	0.600%
13	11.027	1516	1520	1522	rBV2	3935	4919	4.27%	0.468%
14	11.110	1531	1534	1535	rBV3	2068	1940	1.68%	0.185%
15	11.198	1545	1549	1550	rBV3	3017	2806	2.43%	0.267%
16	11.251	1556	1558	1561	rBV4	2225	2280	1.98%	0.217%
17	11.398	1580	1583	1586	rBV	85294	70219	60.91%	6.685%
18	11.421	1586	1587	1590	rVB	6847	3939	3.42%	0.375%
19	11.557	1608	1610	1611	rBV2	2930	2011	1.74%	0.191%
20	11.610	1616	1619	1621	rBV4	3359	4799	4.16%	0.457%
21	11.921	1669	1672	1676	rVB4	16121	18435	15.99%	1.755%
22	12.433	1757	1759	1763	rVB3	14757	15275	13.25%	1.454%
23	12.610	1787	1789	1791	rVB	6893	5364	4.65%	0.511%
24	12.704	1804	1805	1810	rVB5	4247	5157	4.47%	0.491%
25	12.792	1818	1820	1822	rBV3	3811	4046	3.51%	0.385%
26	12.839	1824	1828	1832	rVV3	9172	10387	9.01%	0.989%
27	12.868	1832	1833	1836	rVB2	4170	3006	2.61%	0.286%
28	12.980	1849	1852	1855	rVV	104976	92429	80.17%	8.799%
29	13.015	1855	1858	1859	rVB3	2408	2088	1.81%	0.199%
30	13.104	1871	1873	1875	rVB2	3036	2273	1.97%	0.216%
31	13.162	1881	1883	1886	rVB4	3662	4176	3.62%	0.398%
32	13.204	1889	1890	1891	rBV	3194	1994	1.73%	0.190%
33	13.480	1935	1937	1938	rBV	2072	1518	1.32%	0.145%
34	13.645	1964	1965	1967	rBV	2045	1633	1.42%	0.155%
35	13.839	1996	1998	2003	rVV	3732	2685	2.33%	0.256%
36	13.880	2003	2005	2014	rVB7	5587	10580	9.18%	1.007%

LSC Area Percent Report

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Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
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-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.009	2024	2027	2029	rBV	47752	38859	33.70%	3.699%
38	14.039	2029	2032	2035	rVV	45289	39808	34.53%	3.790%
39	14.062	2035	2036	2038	rVB2	3569	2323	2.01%	0.221%
40	14.198	2056	2059	2063	rBV4	2231	3454	3.00%	0.329%
41	14.421	2096	2097	2101	rBV4	2128	2258	1.96%	0.215%
42	14.657	2135	2137	2142	rVB3	7803	6518	5.65%	0.620%
43	14.804	2160	2162	2166	rVB4	2435	2536	2.20%	0.241%
44	15.004	2194	2196	2199	rVB5	2437	1855	1.61%	0.177%
45	15.080	2207	2209	2212	rVV3	4053	4622	4.01%	0.440%
46	15.109	2212	2214	2216	rVB3	2025	1864	1.62%	0.177%
47	15.145	2218	2220	2223	rVB3	3607	4202	3.64%	0.400%
48	15.368	2254	2258	2259	rBV3	1645	1830	1.59%	0.174%
49	15.392	2259	2262	2264	rVB3	2269	2640	2.29%	0.251%
50	15.439	2268	2270	2271	rBV	2385	1617	1.40%	0.154%
51	15.521	2279	2284	2289	rVB2	24760	33309	28.89%	3.171%
52	15.733	2318	2320	2323	rVB4	1949	1876	1.63%	0.179%
53	15.962	2357	2359	2369	rVB5	3288	5641	4.89%	0.537%
54	16.186	2394	2397	2400	rVB3	1547	1616	1.40%	0.154%
55	16.209	2400	2401	2404	rBV2	1909	1662	1.44%	0.158%
56	16.645	2472	2475	2476	rBV2	2198	1746	1.51%	0.166%
57	16.668	2476	2479	2483	rVV4	1696	3005	2.61%	0.286%
58	16.727	2485	2489	2490	rBV2	1485	1852	1.61%	0.176%
59	16.780	2493	2498	2502	rBV4	2506	5144	4.46%	0.490%
60	16.892	2516	2517	2521	rBV2	1769	2570	2.23%	0.245%
61	17.033	2538	2541	2542	rVB2	2130	1571	1.36%	0.150%
62	17.062	2542	2546	2548	rBV2	1393	2091	1.81%	0.199%
63	17.080	2548	2549	2554	rVB2	1499	1831	1.59%	0.174%
64	17.339	2590	2593	2598	rVB2	1071	1790	1.55%	0.170%
65	17.450	2607	2612	2614	rBV2	1338	2147	1.86%	0.204%
66	17.645	2643	2645	2648	rVB2	1581	1716	1.49%	0.163%
67	17.768	2663	2666	2668	rBV2	1558	1937	1.68%	0.184%

Sum of corrected areas: 1050448

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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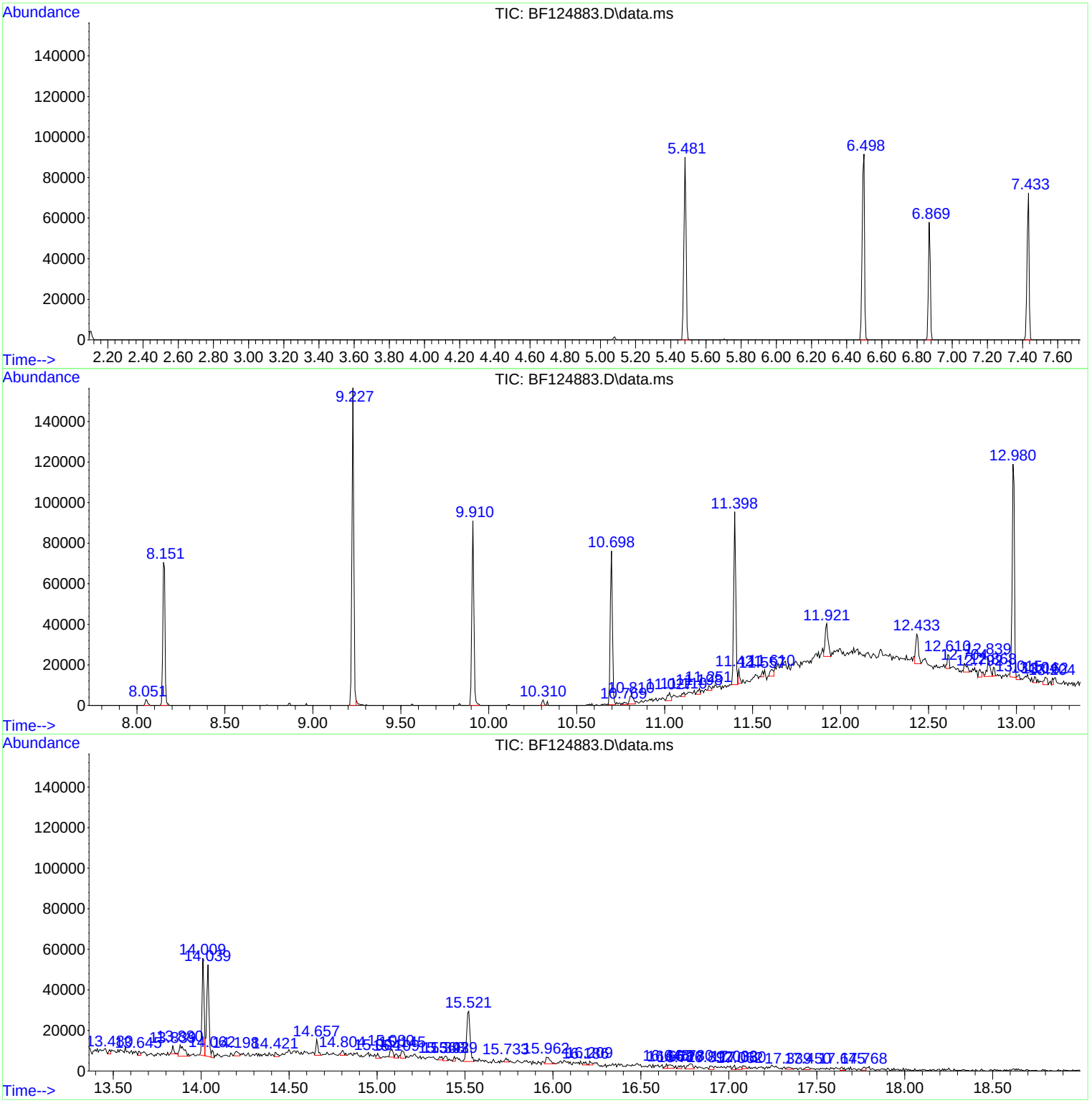
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
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TIC Library : C:\Database\NIST20.L
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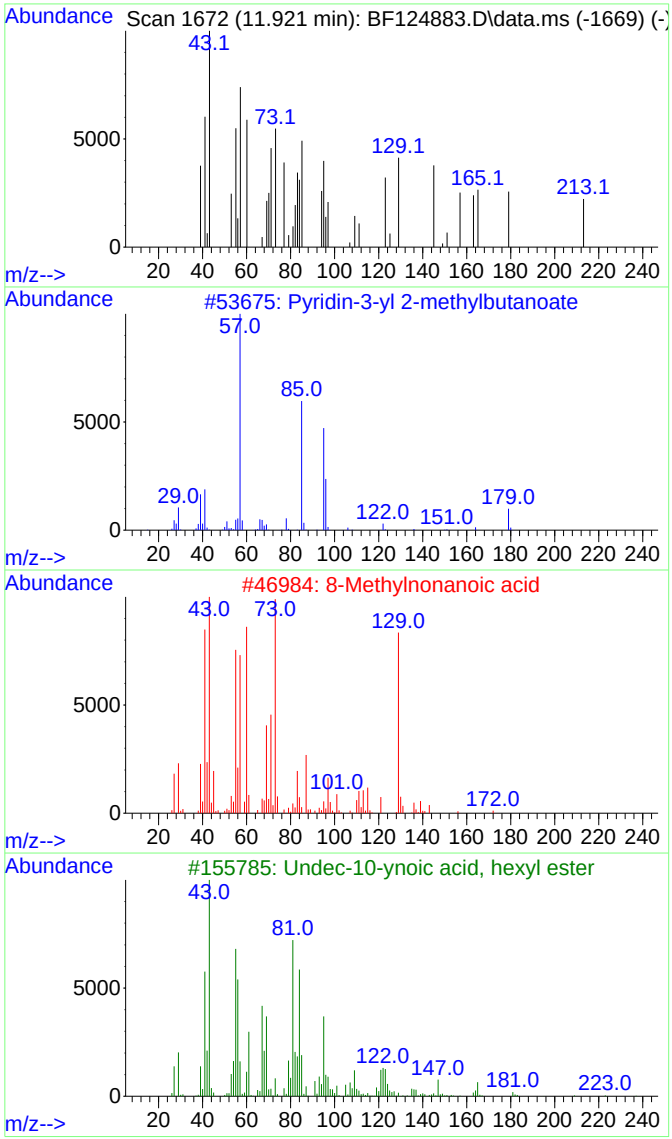
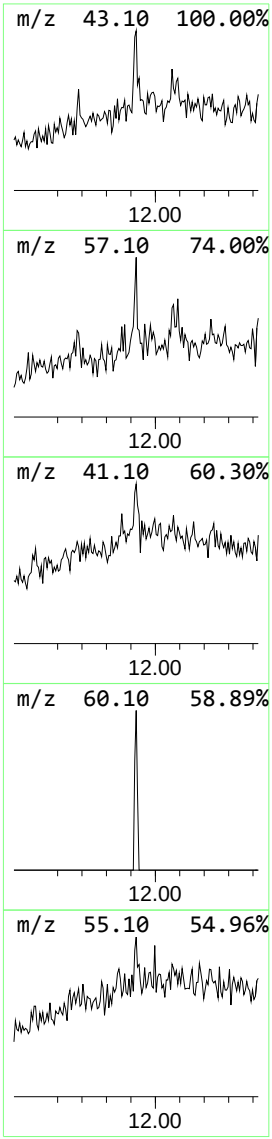
****

Peak Number 1 unknown11.921 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	5.25 ng	18435	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridin-3-yl 2-methylbutanoate	179	C10H13NO2	1000372-73-7	10
2	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	10
3	Undec-10-ynoic acid, hexyl ester	266	C17H30O2	1000406-15-9	10
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	9
5	Undec-10-ynoic acid, isobutyl ester	238	C15H26O2	1000406-15-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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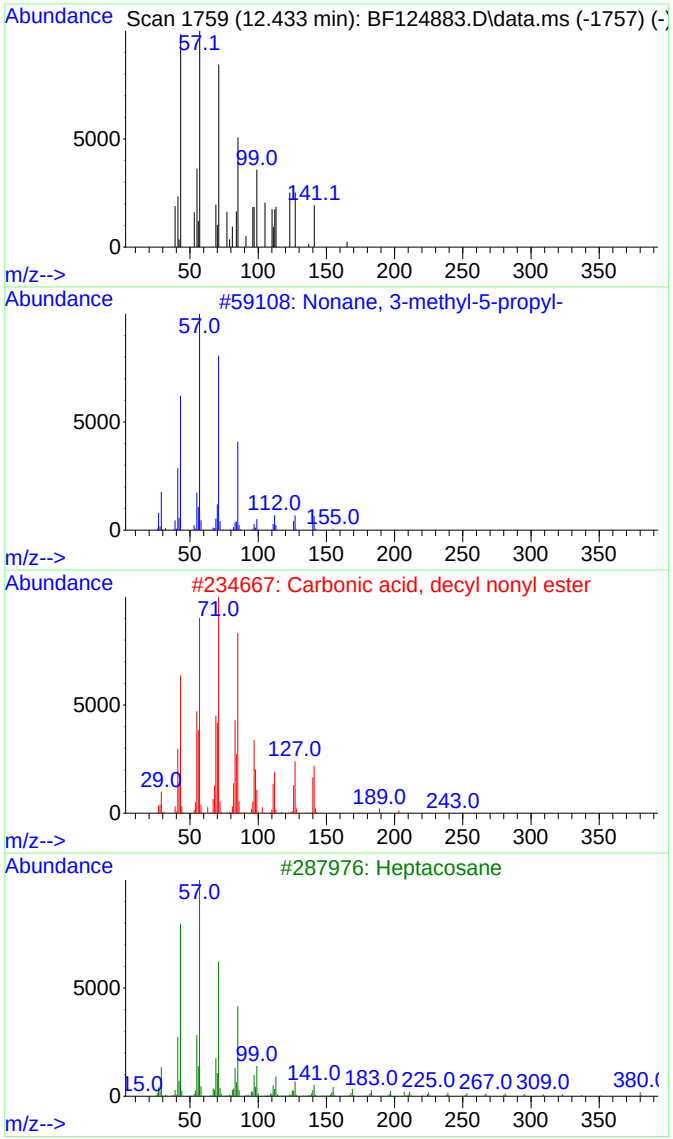
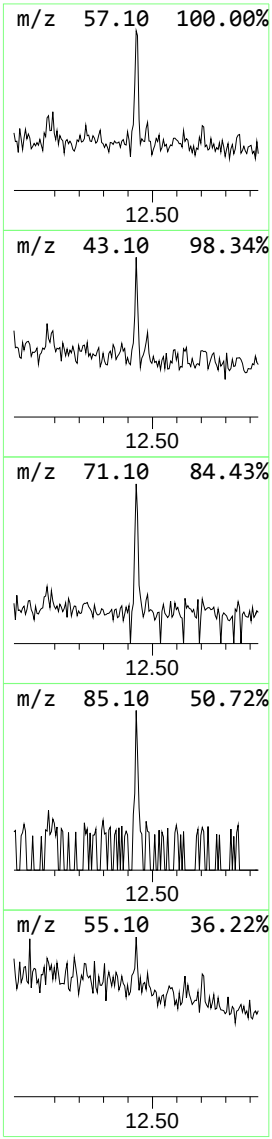
Peak Number 2 Nonane, 3-methyl-5-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	4.35 ng	15275	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	59
2	Carbonic acid, decyl nonyl ester	328	C20H40O3	1000383-15-8	53
3	Heptacosane	380	C27H56	000593-49-7	50
4	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	50
5	Pentacosane	352	C25H52	000629-99-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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Acq On : 30 Jul 2021 18:59
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Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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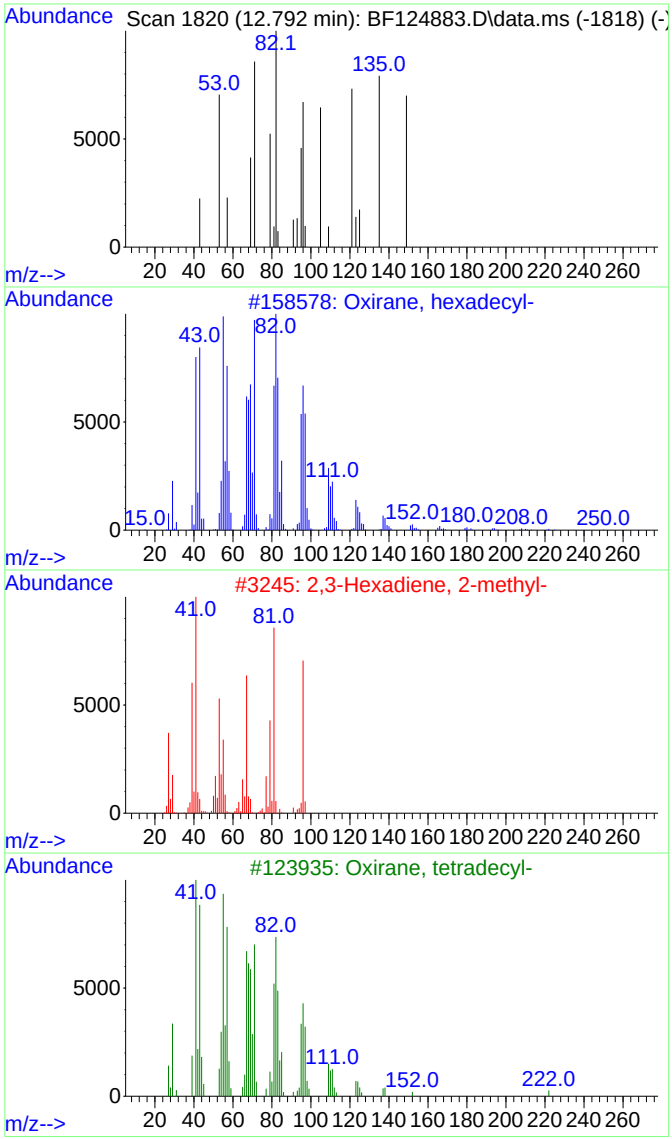
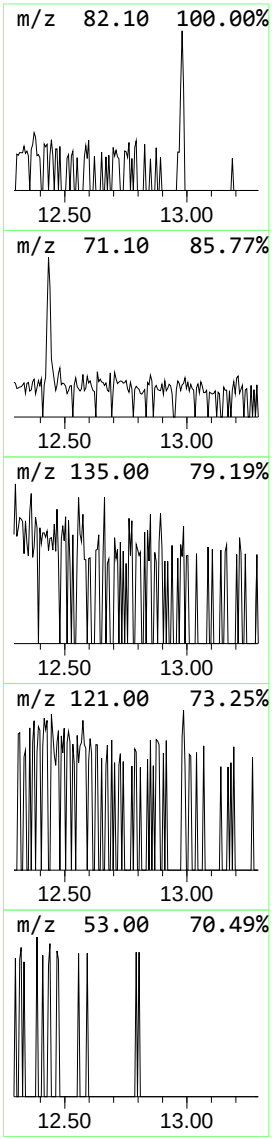
Peak Number 3 unknown12.792 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	2.03 ng	4046	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	12
2	2,3-Hexadiene, 2-methyl-	96	C7H12	029212-09-7	12
3	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	10
4	s(+)-1-Cyano-2-methyl-azetidine	96	C5H8N2	1000143-32-0	9
5	Furan, 2-methyl-	82	C5H6O	000534-22-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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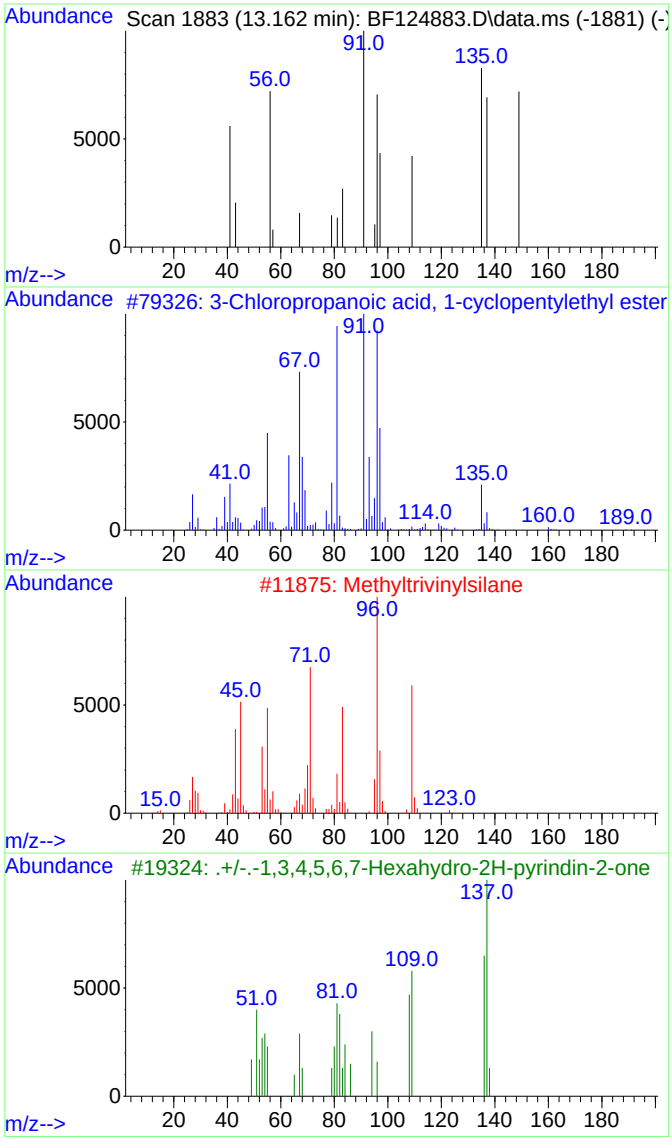
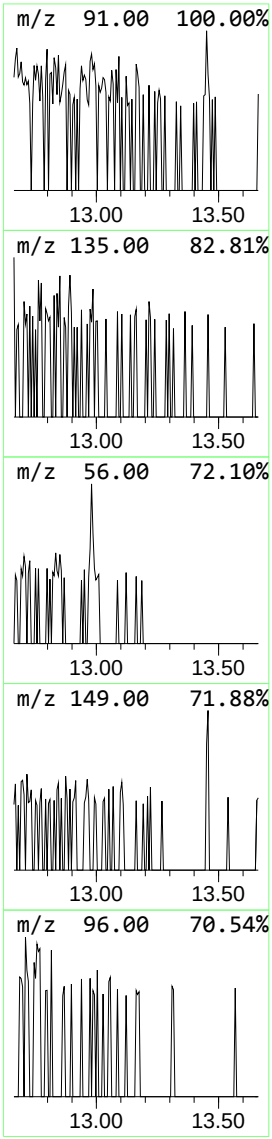
Peak Number 4 unknown13.163 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.10 ng	4176	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropanoic acid, 1-cyclop...	204	C10H17ClO2	1000282-65-5	43
2	Methyltrivinylsilane	124	C7H12Si	018244-95-6	10
3	.+/-.-1,3,4,5,6,7-Hexahydro-2H-p...	137	C8H11NO	010333-13-8	9
4	4-Fluorophenyl isocyanate	137	C7H4FNO	001195-45-5	9
5	1H-Pyrazol-3-amine, 4-methyl-	97	C4H7N3	064781-79-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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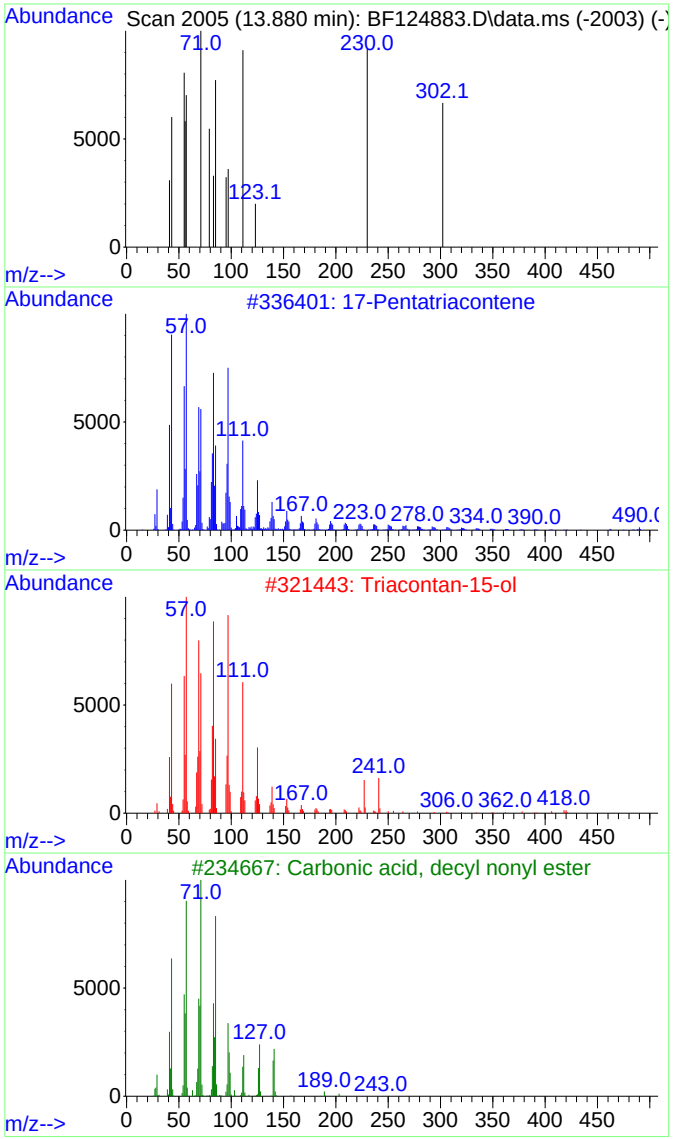
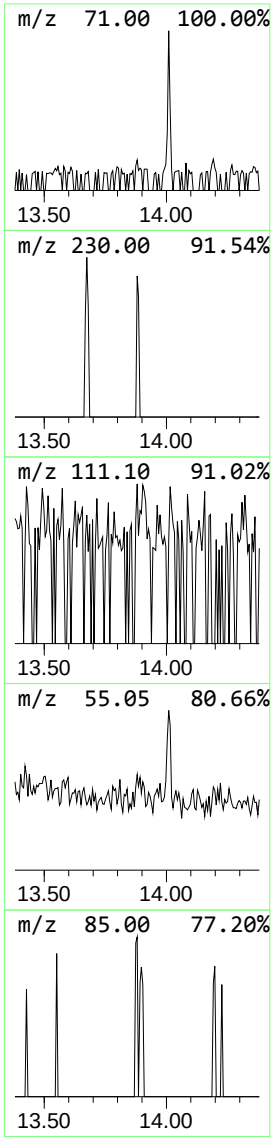
Peak Number 5 unknown13.880 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.32 ng	10580	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	28
2	Triacontan-15-ol	438	C30H62O	031849-26-0	28
3	Carbonic acid, decyl nonyl ester	328	C20H40O3	1000383-15-8	27
4	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	27
5	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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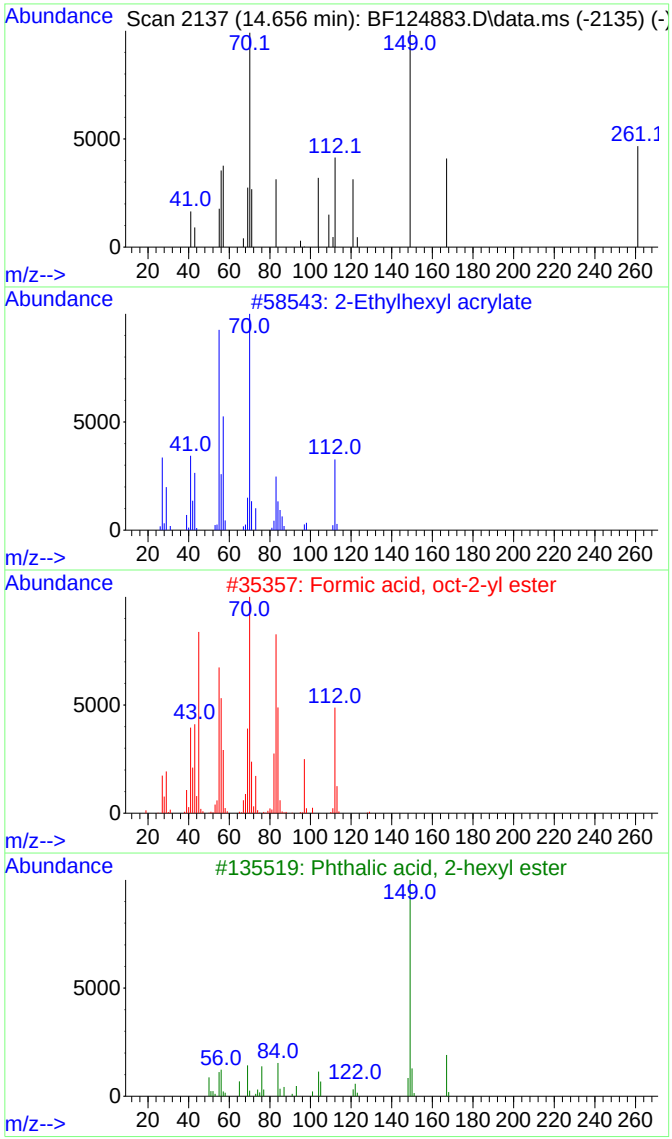
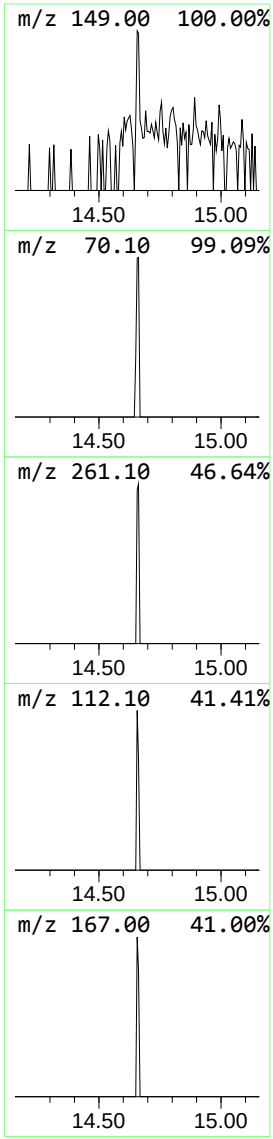
Peak Number 6 unknown14.656 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.656	3.27 ng	6518	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl acrylate	184	C11H20O2	000103-11-7	17
2	Formic acid, oct-2-yl ester	158	C9H18O2	1000368-94-5	12
3	Phthalic acid, 2-hexyl ester	250	C14H18O4	079107-80-5	12
4	Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	12
5	Phthalic acid, but-3-yn-2-yl 2-e...	330	C20H26O4	1000315-76-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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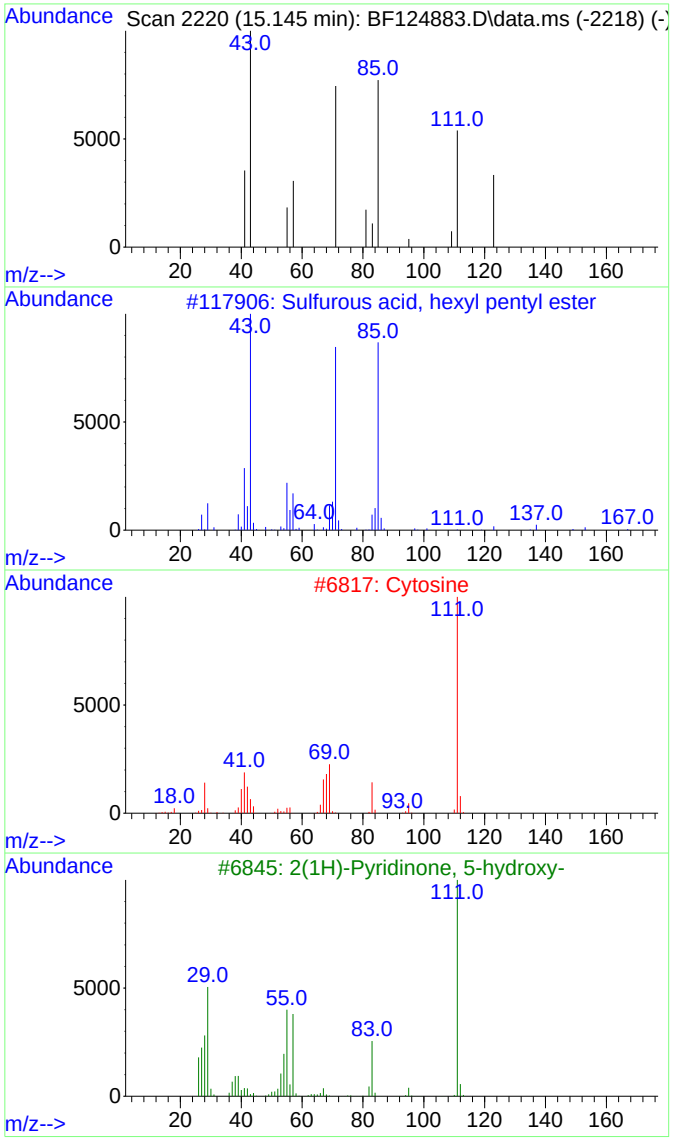
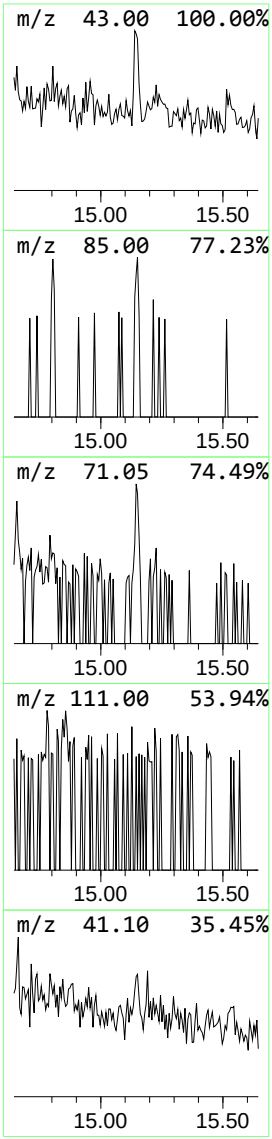
Peak Number 7 unknown15.145 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.52 ng	4202	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	33
2	Cytosine	111	C4H5N3O	000071-30-7	7
3	2(1H)-Pyridinone, 5-hydroxy-	111	C5H5NO2	005154-01-8	7
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
5	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

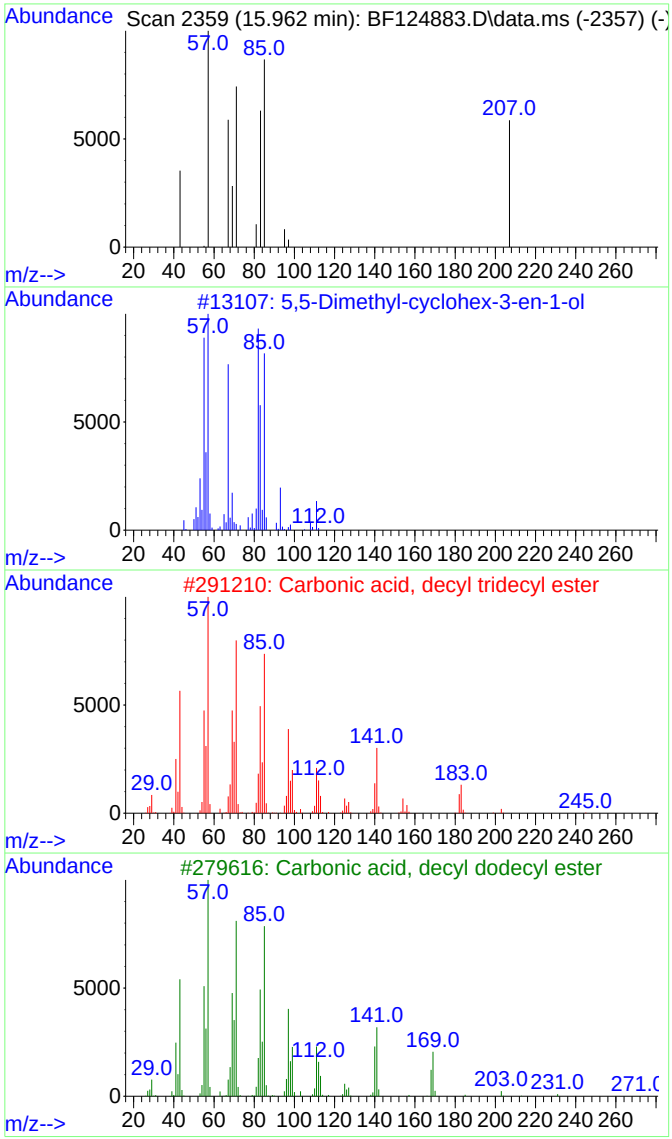
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

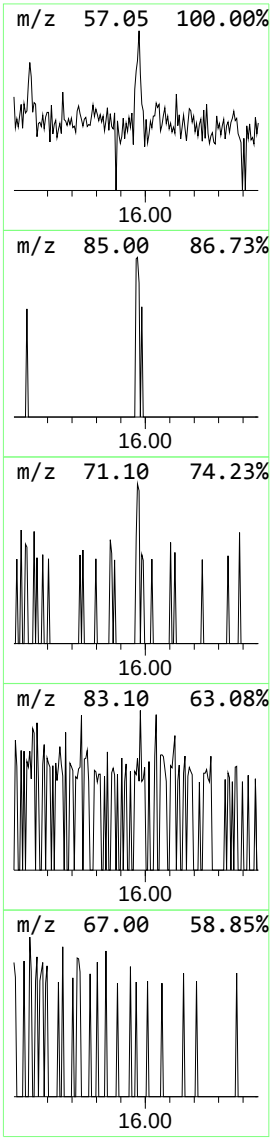
****

Peak Number 8 unknown15.962 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.962	3.39 ng	5641	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dimethyl-cyclohex-3-en-1-ol	126	C8H14O	082299-68-1	37
2	Carbonic acid, decyl tridecyl ester	384	C24H48O3	1000383-16-2	36
3	Carbonic acid, decyl dodecyl ester	370	C23H46O3	1000383-16-1	36
4	Succinic acid, dodec-2-en-1-yl t...	368	C21H36O5	1000390-72-8	28
5	Oxalic acid, 6-ethyloct-3-yl hep...	328	C19H36O4	1000309-34-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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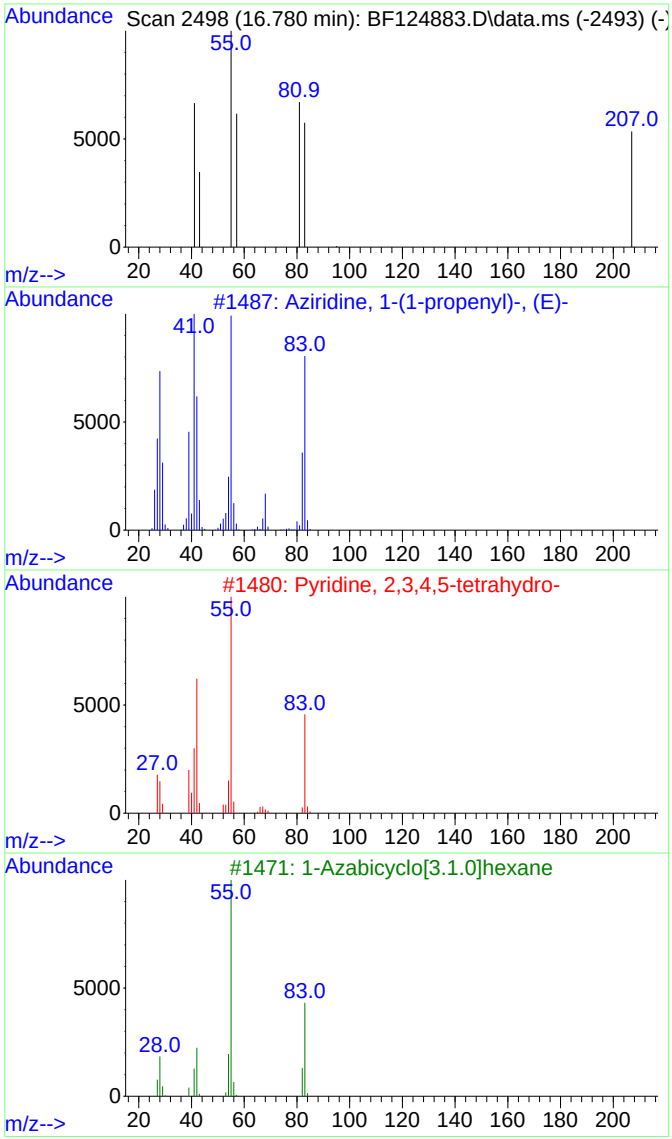
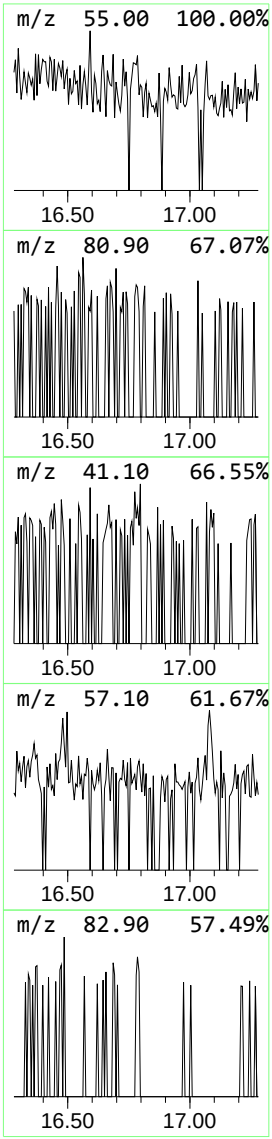
Peak Number 9 unknown16.780 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	3.09 ng	5144	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
2	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
3	1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	4
4	6-Nitro-8-methoxy-2H-chromene	207	C10H9NO4	062063-07-4	2
5	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124883.D
Acq On : 30 Jul 2021 18:59
Operator : JU/CG
Sample : M3238-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 282

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown11.921	11.921	5.3	ng	18435	4	11.398	70219	20.0
Nonane, 3-methy...	12.433	4.3	ng	15275	4	11.398	70219	20.0
unknown12.792	12.792	2.0	ng	4046	5	14.039	39808	20.0
unknown13.163	13.163	2.1	ng	4176	5	14.039	39808	20.0
unknown13.880	13.880	5.3	ng	10580	5	14.039	39808	20.0
unknown14.656	14.656	3.3	ng	6518	5	14.039	39808	20.0
unknown15.145	15.145	2.5	ng	4202	6	15.521	33309	20.0
unknown15.962	15.962	3.4	ng	5641	6	15.521	33309	20.0
unknown16.780	16.780	3.1	ng	5144	6	15.521	33309	20.0