LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121218.D
Acq On : 6 Aug 2020 23:14
Operator : JU/CG
Sample : L3573-03 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-016-B

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-BF071620.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	4.340	379	383	392	rBV	180104	226353	13.43%	1.062%
2	4.987	487	493	496	rBV	1064569	1200831	71.24%	5.636%
3	5.404	560	564	574	rBV	1297973	1271468	75.43%	5.968%
4	6.428	734	738	753	rBV	1333517	1299530	77.10%	6.099%
5	6.628	768	772	777	rBV4	21798	31634	1.88%	0.148%
6	6.792	796	800	807	rBV	1001671	801545	47.55%	3.762%
7	7.057	841	845	850	rBV	14241	18732	1.11%	0.088%
8	7.351	892	895	906	rBV	841106	880301	52.23%	4.132%
9	8.075	1015	1018	1031	rVB	1129744	1067854	63.35%	5.012%
10	8.669	1116	1119	1122	rBV	23403	19714	1.17%	0.093%
11	9.098	1189	1192	1195	rBV2	25912	20655	1.23%	0.097%
12	9.151	1197	1201	1211	rBV	1817977	1685533	100.00%	7.911%
13	9.233	1212	1215	1218	rVB2	46094	42766	2.54%	0.201%
14	9.551	1265	1269	1273	rBV	211530	247044	14.66%	1.159%
15	9.610	1277	1279	1283	rVB4	18329	18949	1.12%	0.089%
16	9.692	1290	1293	1298	rBV	55306	66495	3.95%	0.312%
17	9.763	1303	1305	1310	rVB	39495	36419	2.16%	0.171%
18	9.833	1313	1317	1332	rVV	1427738	1323141	78.50%	6.210%
19	9.939	1332	1335	1339	rVB4	19235	23498	1.39%	0.110%
20	10.033	1348	1351	1356	rVB3	19837	28033	1.66%	0.132%
21	10.074	1356	1358	1363	rVB3	14382	19757	1.17%	0.093%
22	10.151	1368	1371	1374	rBV2	24142	32399	1.92%	0.152%
23	10.239	1383	1386	1388	rBV2	39214	41396	2.46%	0.194%
24	10.263	1388	1390	1393	rVB2	48090	35135	2.08%	0.165%
25	10.380	1407	1410	1417	rBV4	18257	36264	2.15%	0.170%
26	10.486	1426	1428	1432	rVB2	26377	27294	1.62%	0.128%
27	10.533	1434	1436	1440	rVB3	17066	21666	1.29%	0.102%
28	10.621	1448	1451	1463	rVB	895664	980499	58.17%	4.602%
29	10.745	1468	1472	1479	rVB2	63216	108896	6.46%	0.511%
30	11.186	1544	1547	1549	rBV	36931	32488	1.93%	0.152%
31	11.216	1549	1552	1558	rVB	53878	60657	3.60%	0.285%
32	11.321	1566	1570	1572	rBV	1362512	1203529	71.40%	5.649%
33	11.345	1572	1574	1578	rVV	218309	209711	12.44%	0.984%
34	11.398	1580	1583	1586	rVV	79246	77878	4.62%	0.366%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121218.D
Acq On : 6 Aug 2020 23:14
Operator : JU/CG
Sample : L3573-03 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-016-B

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.433	1586	1589	1592	rVV2	18898	19367	1.15%	0.091%
36	11.563	1607	1611	1617	rBV5	25122	48704	2.89%	0.229%
37	11.610	1617	1619	1622	rVB2	37384	34571	2.05%	0.162%
38	11.821	1652	1655	1658	rBV2	54899	54920	3.26%	0.258%
39	11.851	1658	1660	1663	rVB	77000	54574	3.24%	0.256%
40	11.898	1666	1668	1671	rBV	22057	21426	1.27%	0.101%
41	11.933	1671	1674	1677	rBV	110323	107705	6.39%	0.506%
42	12.021	1686	1689	1692	rVB	44850	42085	2.50%	0.198%
43	12.057	1692	1695	1698	rBV2	29812	26236	1.56%	0.123%
44	12.116	1703	1705	1707	rBV	40482	38756	2.30%	0.182%
45	12.251	1725	1728	1729	rBV	34170	35299	2.09%	0.166%
46	12.298	1733	1736	1738	rBV2	74492	78094	4.63%	0.367%
47	12.374	1745	1749	1751	rBV	67782	75952	4.51%	0.356%
48	12.410	1752	1755	1757	rVV	77869	81652	4.84%	0.383%
49	12.457	1761	1763	1767	rBV2	40280	47969	2.85%	0.225%
50	12.533	1773	1776	1780	rBV	681063	584257	34.66%	2.742%
51	12.686	1800	1802	1805	rBV2	39074	43090	2.56%	0.202%
52	12.763	1809	1815	1821	rBV	655479	736333	43.69%	3.456%
53	12.904	1835	1839	1846	rVB	1709256	1585655	94.07%	7.442%
54	13.092	1868	1871	1874	rVB	134895	141734	8.41%	0.665%
55	13.133	1876	1878	1880	rVV2	51942	49475	2.94%	0.232%
56	13.157	1880	1882	1885	rVB	97217	73205	4.34%	0.344%
57	13.198	1886	1889	1891	rVV2	69675	72720	4.31%	0.341%
58	13.810	1991	1993	2001	rVB4	178035	263746	15.65%	1.238%
59	13.962	2014	2019	2022	rBV2	1205609	1484615	88.08%	6.968%
60	13.986	2022	2023	2029	rVB	355363	281191	16.68%	1.320%
61	14.998	2192	2195	2202	rVB	362798	624987	37.08%	2.933%
62	15.356	2253	2256	2262	rVB	304333	350134	20.77%	1.643%
63	15.421	2263	2267	2275	rVB	730165	1049835	62.29%	4.927%

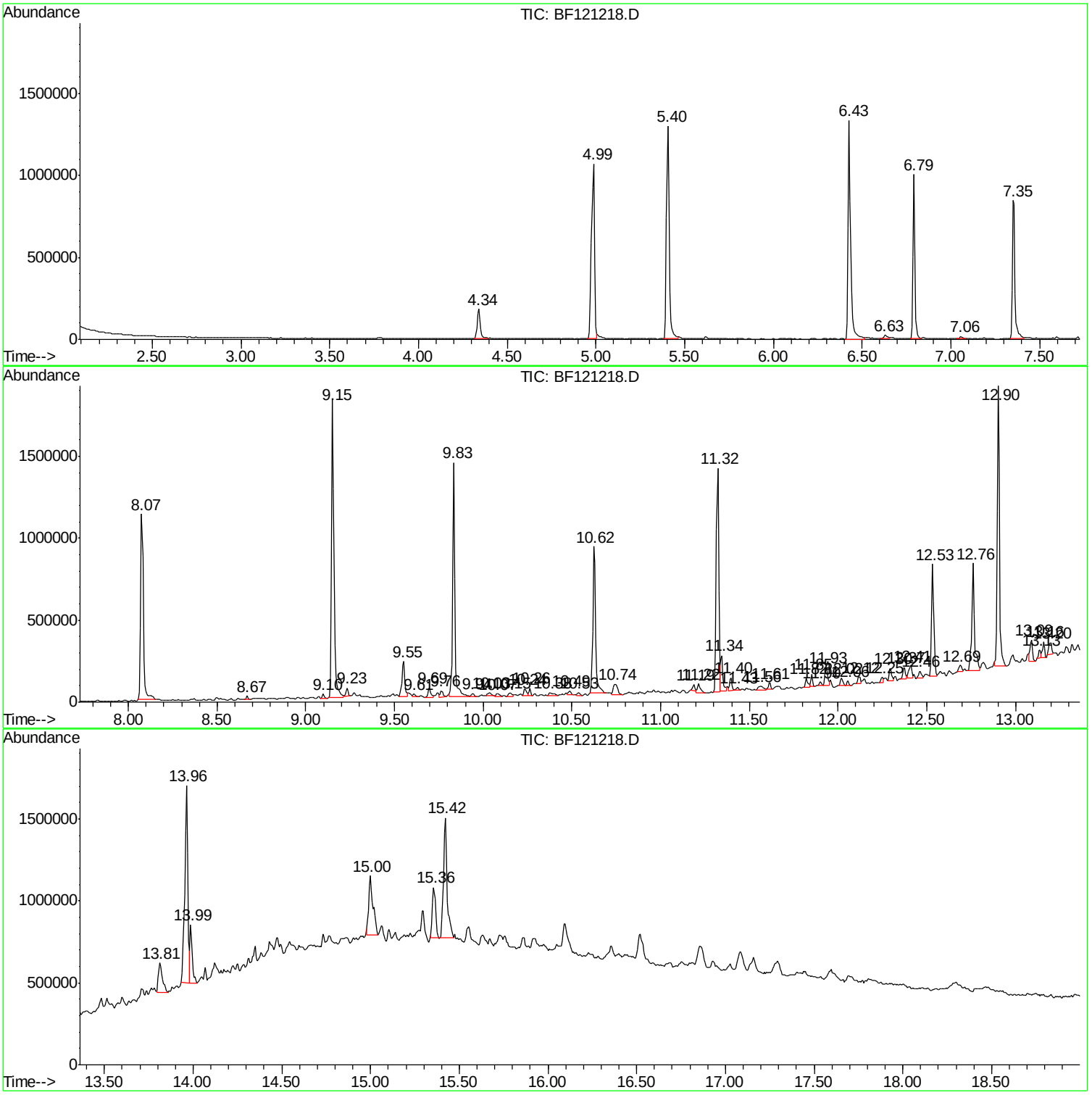
Sum of corrected areas: 21306351

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121218.D
Acq On : 6 Aug 2020 23:14
Operator : JU/CG
Sample : L3573-03 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-03-016-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121218.D
Acq On : 6 Aug 2020 23:14
Operator : JU/CG
Sample : L3573-03 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-016-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

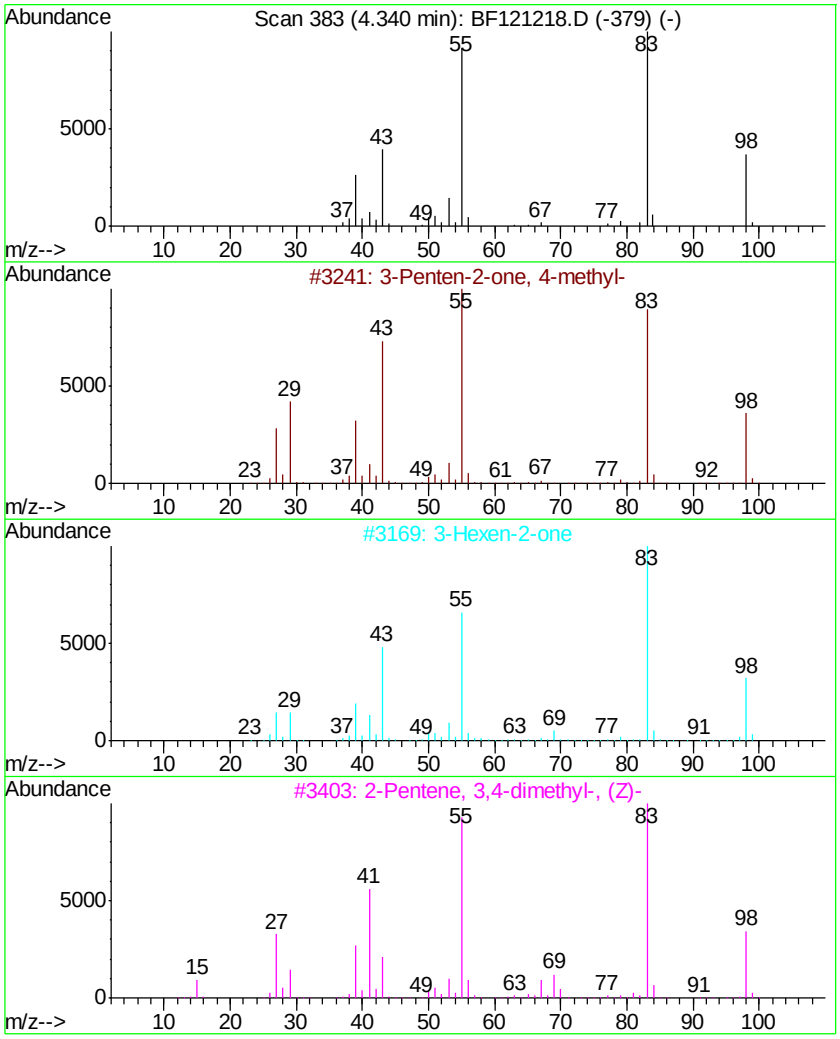
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

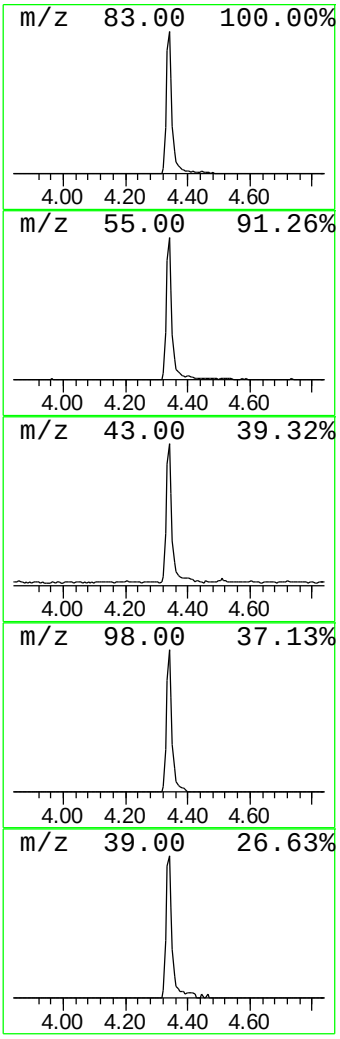
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.34	5.65 ng	226353	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121218.D
Acq On : 6 Aug 2020 23:14
Operator : JU/CG
Sample : L3573-03 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-016-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

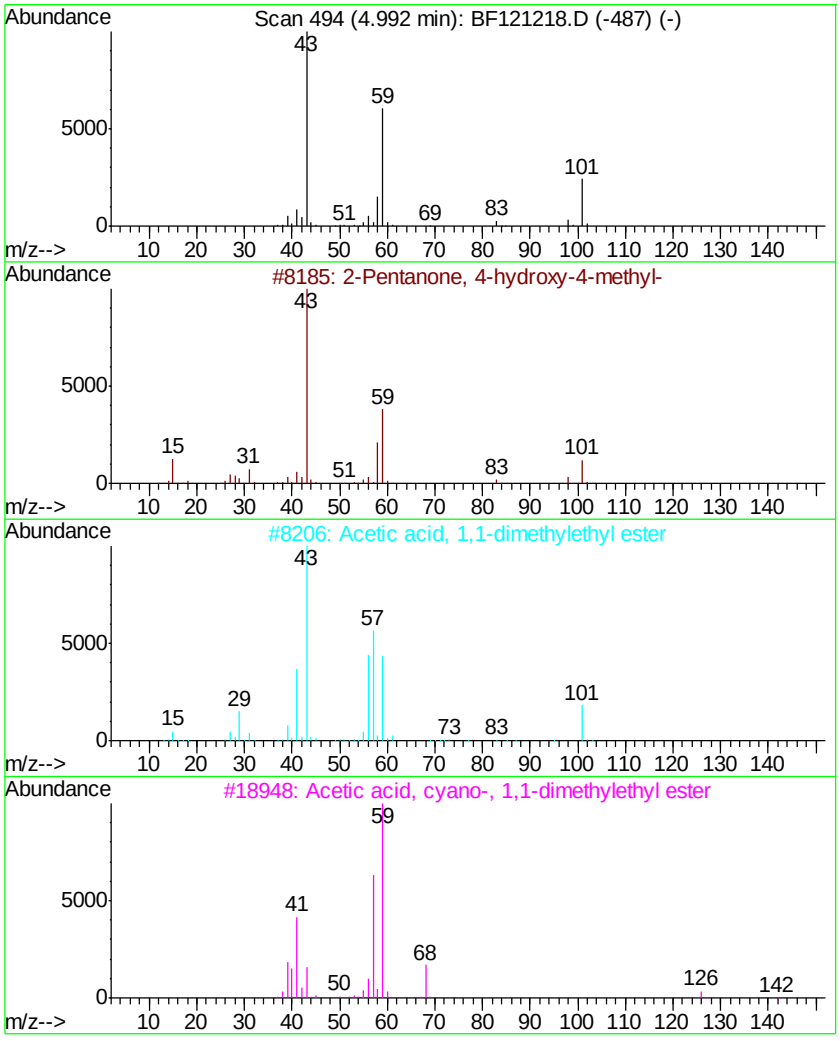
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

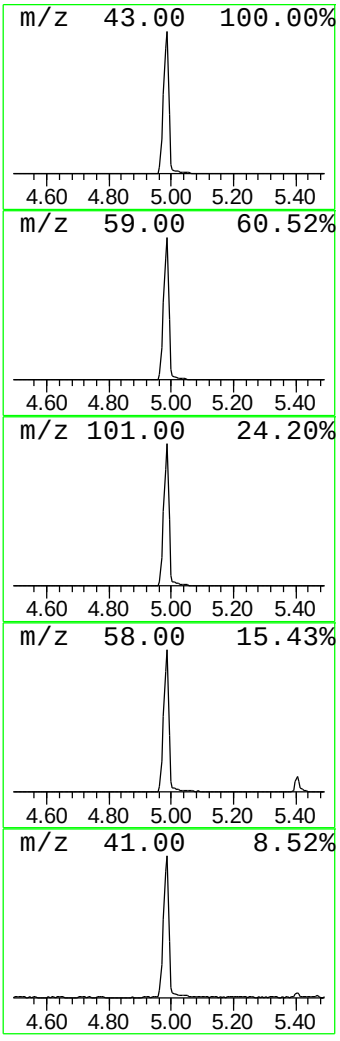
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	29.96 ng	1200830	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121218.D
Acq On : 6 Aug 2020 23:14
Operator : JU/CG
Sample : L3573-03 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-016-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

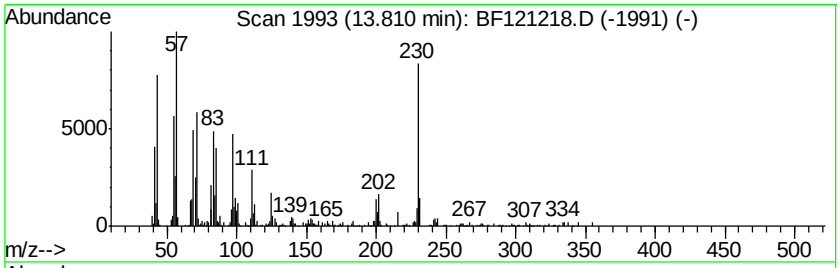
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

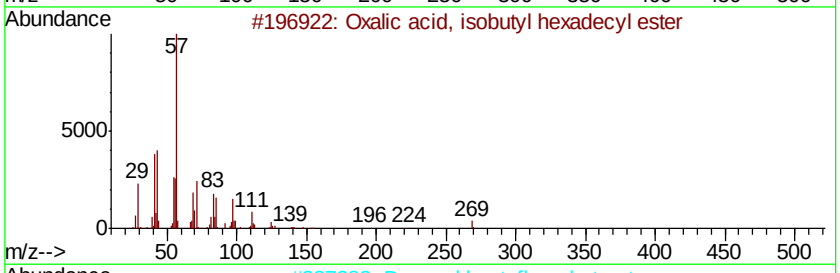
****

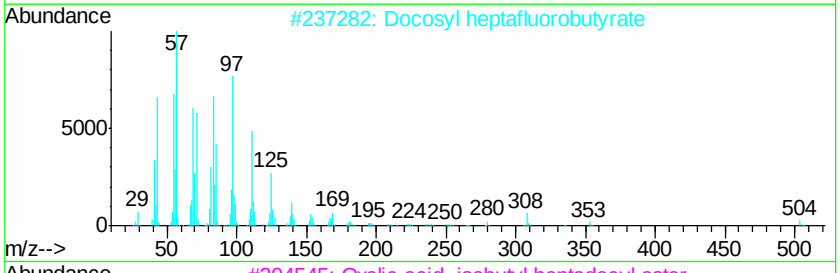
Peak Number 3 Oxalic acid, isobutyl hexad... Concentration Rank 3

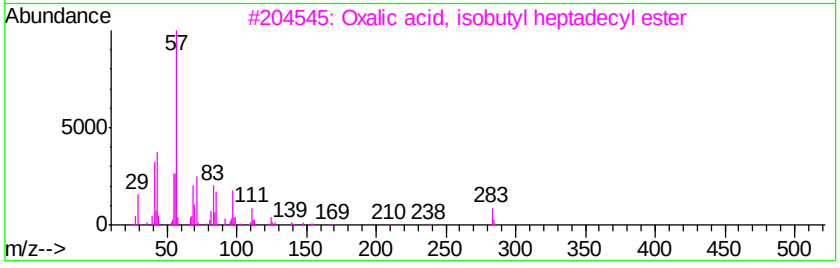
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.55 ng	263746	Chrysene-d12	13.96

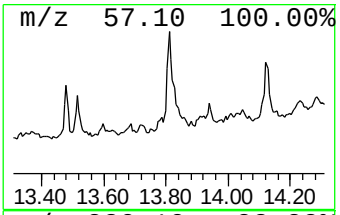
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	53
2	Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	53
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	53
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	53
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	49

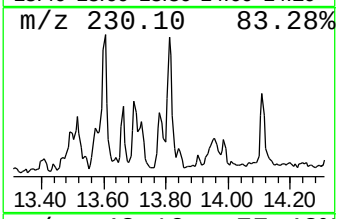


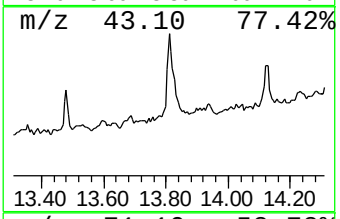


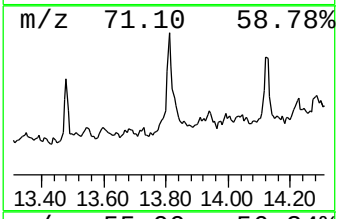


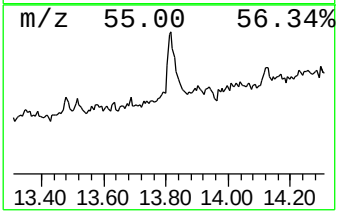












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080620\
Data File : BF121218.D
Acq On : 6 Aug 2020 23:14
Operator : JU/CG
Sample : L3573-03 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-016-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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
3-Penten-2-one, 4...	4.34	5.7	ng	226353	1	6.79	801545	20.0
2-Pentanone, 4-hy...	4.99	30.0	ng	1200830	1	6.79	801545	20.0
Oxalic acid, isob...	13.81	3.5	ng	263746	5	13.96	1484620	20.0