LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126244.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	16	20	26	rVB	83476	102213	2.34%	0.291%
2	5.028	494	500	508	rVB	585042	717251	16.41%	2.045%
3	5.428	563	568	571	rBV	4183681	4324094	98.93%	12.329%
4	5.828	633	636	640	rVB	82457	71570	1.64%	0.204%
5	6.439	735	740	751	rBV	3727273	4370711	100.00%	12.462%
6	6.816	800	804	808	rBV	1549919	1231793	28.18%	3.512%
7	7.375	894	899	902	rBV	2694342	2797226	64.00%	7.975%
8	7.586	932	935	939	rBV2	45193	46116	1.06%	0.131%
9	8.004	1002	1006	1014	rBV	244345	233816	5.35%	0.667%
10	8.098	1018	1022	1025	rBV	1962133	1568531	35.89%	4.472%
11	8.910	1154	1160	1163	rVB	80502	61233	1.40%	0.175%
12	9.175	1201	1205	1209	rBV	3926101	3577811	81.86%	10.201%
13	9.275	1217	1222	1224	rBV2	66297	92799	2.12%	0.265%
14	9.304	1224	1227	1236	rVB	209333	267829	6.13%	0.764%
15	9.510	1259	1262	1265	rBV2	58405	59024	1.35%	0.168%
16	9.669	1286	1289	1295	rBV2	69366	97202	2.22%	0.277%
17	9.851	1313	1320	1323	rBV	1479306	1407763	32.21%	4.014%
18	9.886	1323	1326	1331	rVB	427329	336093	7.69%	0.958%
19	10.057	1352	1355	1358	rBV	258994	193326	4.42%	0.551%
20	10.269	1387	1391	1393	rBV2	99084	98913	2.26%	0.282%
21	10.398	1410	1413	1419	rVB	364544	298885	6.84%	0.852%
22	10.469	1419	1425	1426	rBV2	36808	48433	1.11%	0.138%
23	10.557	1438	1440	1444	rVB2	87197	79988	1.83%	0.228%
24	10.639	1450	1454	1457	rBV	2078887	1828040	41.82%	5.212%
25	10.763	1473	1475	1476	rBV	75330	58744	1.34%	0.167%
26	10.780	1476	1478	1483	rVB2	97572	89347	2.04%	0.255%
27	10.945	1502	1506	1509	rBV3	43925	49813	1.14%	0.142%
28	11.186	1544	1547	1550	rBV3	34809	48067	1.10%	0.137%
29	11.233	1553	1555	1561	rVB2	101141	125399	2.87%	0.358%
30	11.304	1563	1567	1569	rBV	121771	95796	2.19%	0.273%
31	11.339	1569	1573	1575	rVV	1196145	1202306	27.51%	3.428%
32	11.363	1575	1577	1580	rVV	971758	745807	17.06%	2.126%
33	11.410	1580	1585	1588	rVB	110271	124932	2.86%	0.356%
34	11.510	1600	1602	1608	rVB	38119	44649	1.02%	0.127%
35	11.639	1621	1624	1627	rBV2	69962	59946	1.37%	0.171%
36	11.739	1638	1641	1646	rVB2	103749	92575	2.12%	0.264%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.839	1654	1658	1660	rBV	82254	77437	1.77%	0.221%
38	11.863	1660	1662	1666	rVB	220263	205630	4.70%	0.586%
39	11.904	1666	1669	1672	rBV2	61128	60845	1.39%	0.173%
40	11.951	1673	1677	1679	rBV2	131851	137950	3.16%	0.393%
41	12.045	1690	1693	1696	rBV2	57472	46533	1.06%	0.133%
42	12.133	1705	1708	1710	rBV	57019	58360	1.34%	0.166%
43	12.327	1737	1741	1745	rBV3	56359	91092	2.08%	0.260%
44	12.380	1748	1750	1755	rVV3	63059	89553	2.05%	0.255%
45	12.439	1755	1760	1763	rVB4	69160	102409	2.34%	0.292%
46	12.545	1775	1778	1781	rBV	656037	552323	12.64%	1.575%
47	12.651	1793	1796	1800	rBV6	26635	44194	1.01%	0.126%
48	12.774	1811	1817	1820	rBV	588164	598367	13.69%	1.706%
49	12.921	1838	1842	1846	rVB	2694466	2458378	56.25%	7.009%
50	13.104	1870	1873	1876	rVB	109309	92399	2.11%	0.263%
51	13.168	1880	1884	1887	rVB2	88439	86554	1.98%	0.247%
52	13.204	1887	1890	1893	rBV2	57385	59934	1.37%	0.171%
53	13.721	1974	1978	1981	rBV2	54136	72606	1.66%	0.207%
54	13.833	1991	1997	2005	rBV3	286860	418721	9.58%	1.194%
55	13.968	2015	2020	2023	rBV2	1135207	1298160	29.70%	3.701%
56	13.998	2023	2025	2030	rVB	221463	187501	4.29%	0.535%
57	14.286	2069	2074	2078	rBV5	37320	81033	1.85%	0.231%
58	14.657	2135	2137	2142	rBV5	43157	75576	1.73%	0.215%
59	14.833	2164	2167	2172	rBV2	230532	253001	5.79%	0.721%
60	14.939	2182	2185	2189	rVB2	53324	57370	1.31%	0.164%
61	14.998	2191	2195	2198	rBV	130222	179484	4.11%	0.512%
62	15.292	2242	2245	2252	rVB	96376	128618	2.94%	0.367%
63	15.357	2252	2256	2259	rBV	102752	123725	2.83%	0.353%
64	15.415	2262	2266	2271	rBV	593227	739466	16.92%	2.108%
65	15.898	2346	2348	2353	rVB2	39309	47504	1.09%	0.135%

Sum of corrected areas: 35072764

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
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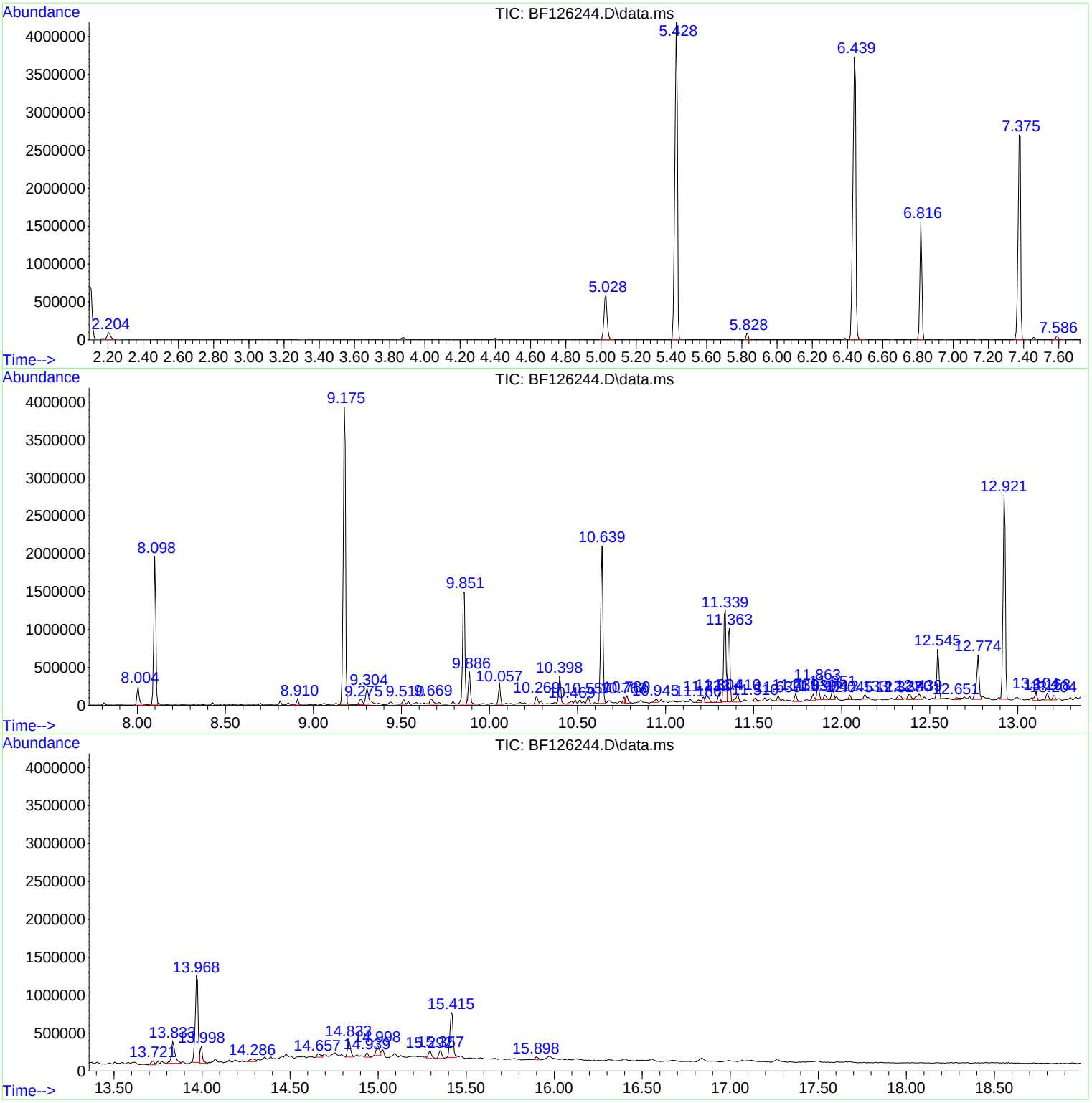
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
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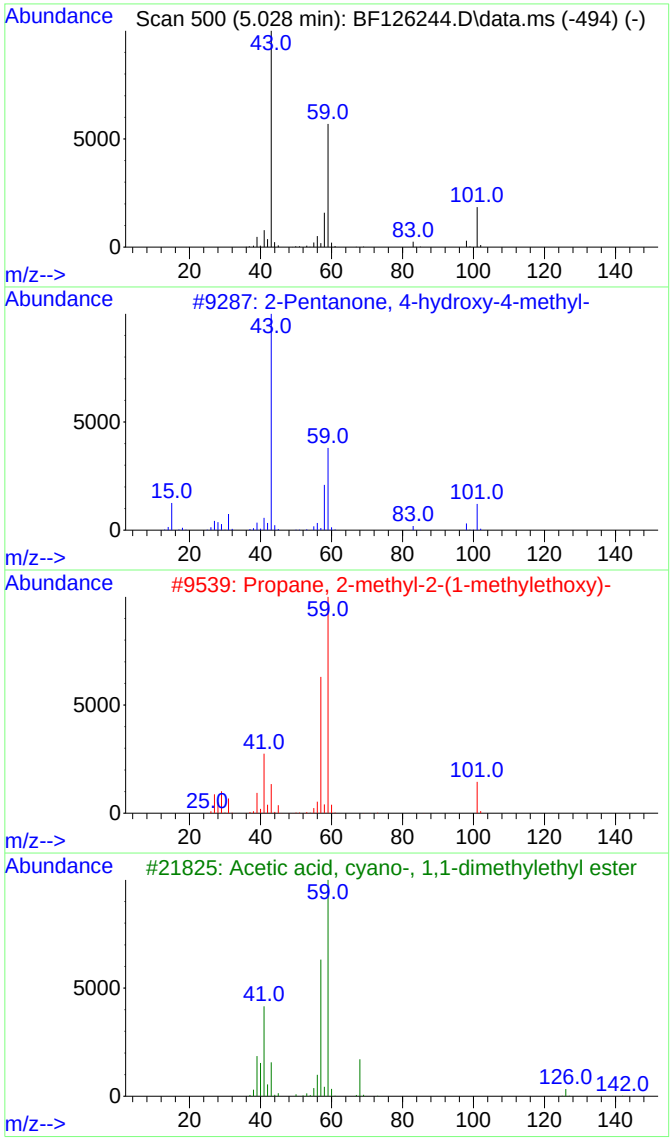
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

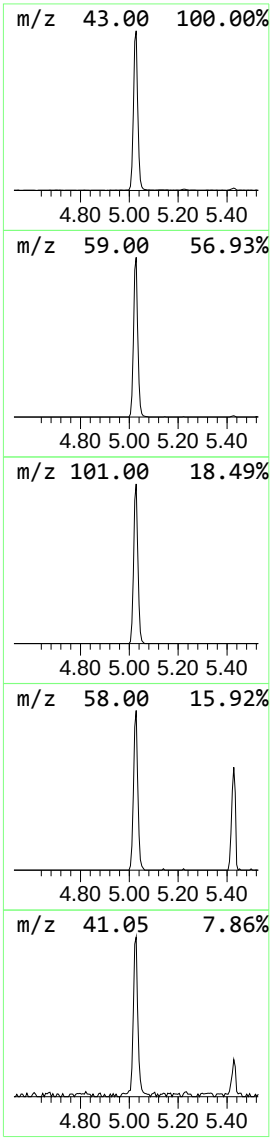
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	11.65 ng	717251	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

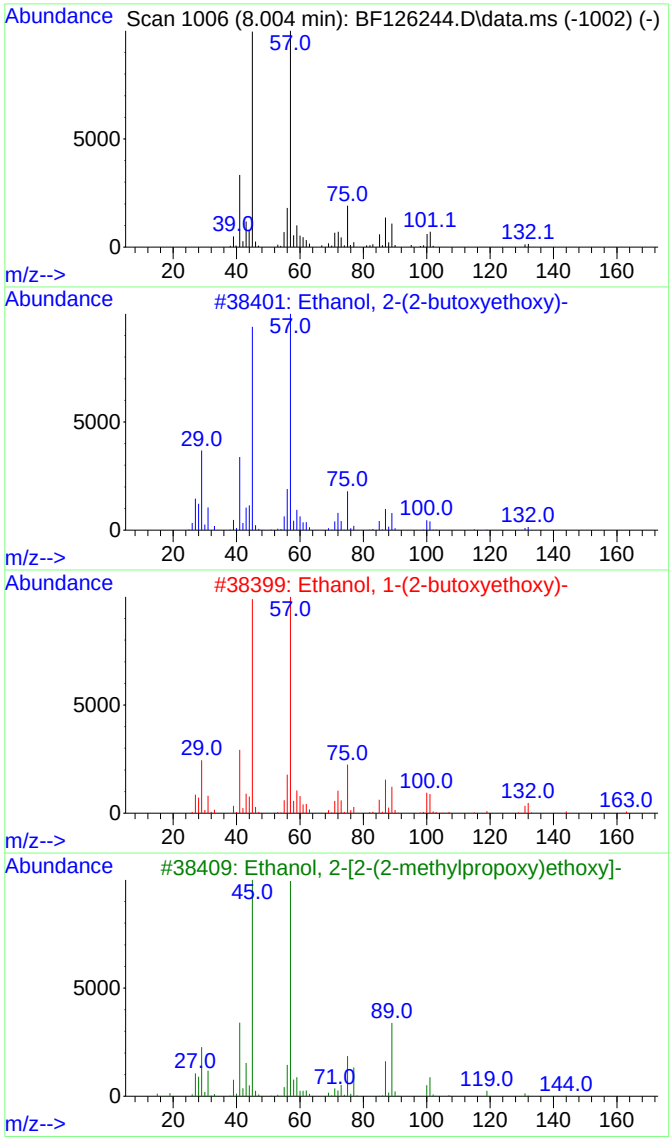
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

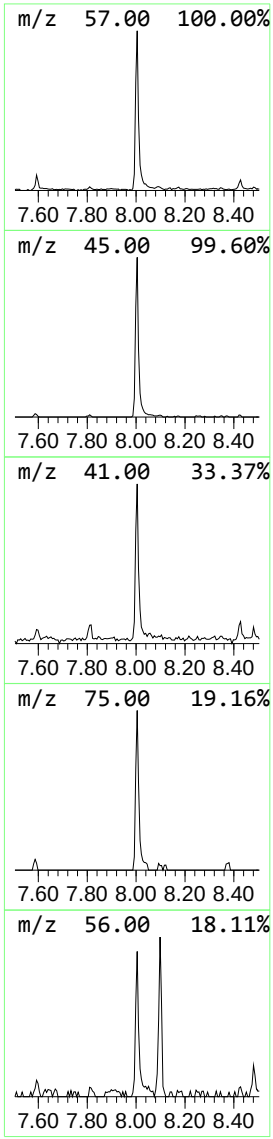
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	2.98 ng	233816	Naphthalene-d8	8.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

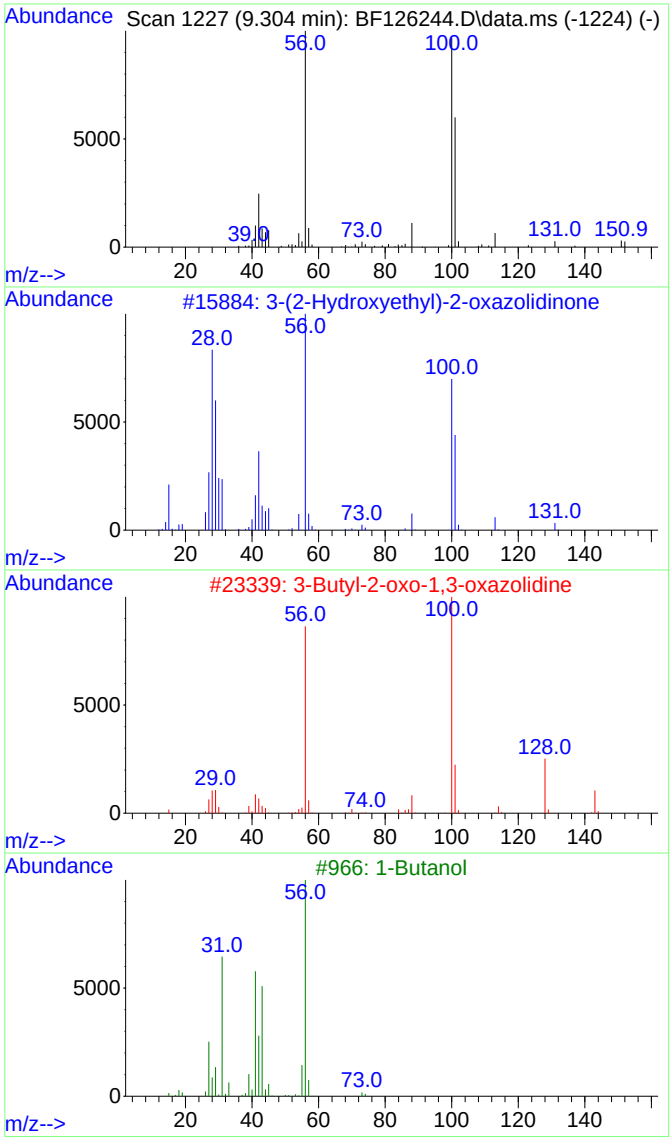
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

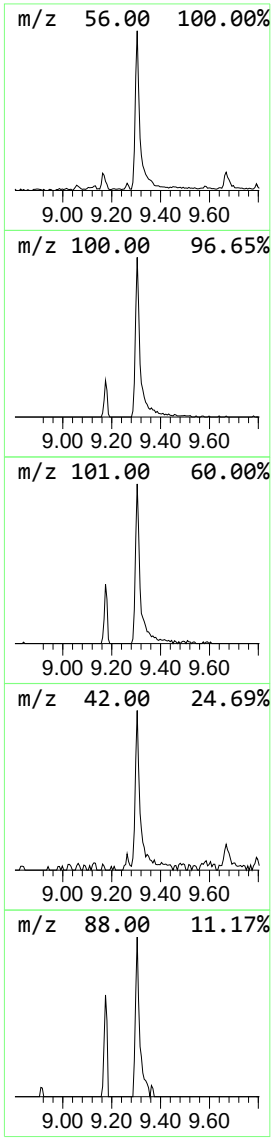
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.304	3.81 ng	267829	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	91
2	3-Butyl-2-oxo-1,3-oxazolidine	143	C7H13NO2	023288-01-9	50
3	1-Butanol	74	C4H10O	000071-36-3	27
4	N-(3-Hydoxypropyl)morpholine	145	C7H15NO2	1000425-83-2	25
5	4-Hydroxypiperidine	101	C5H11NO	005382-16-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

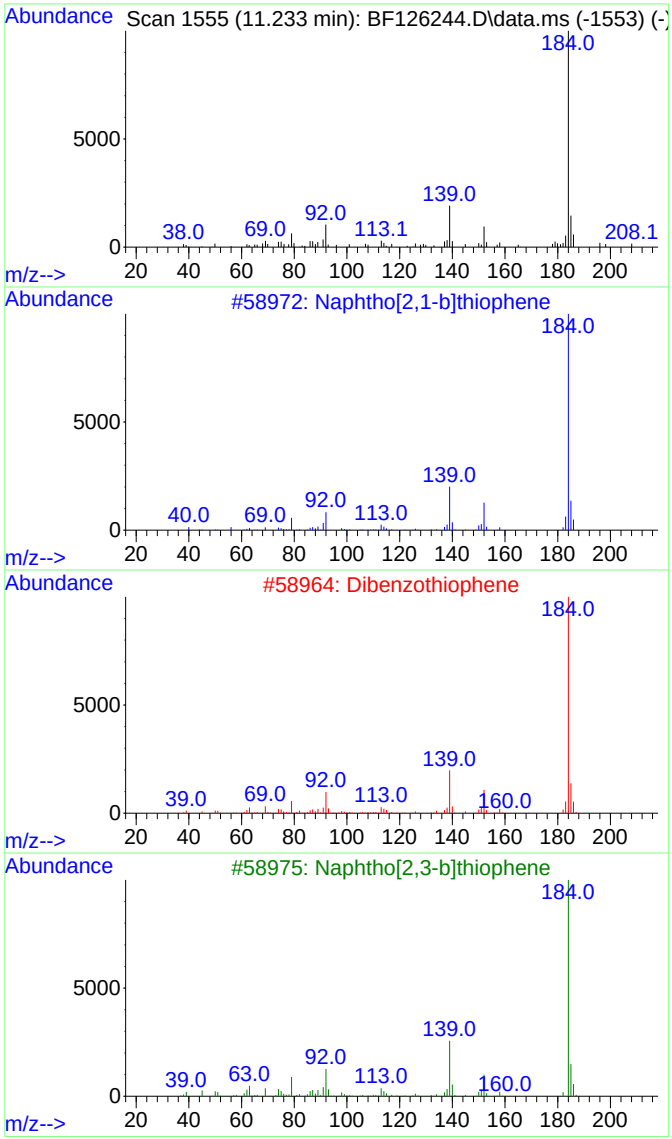
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

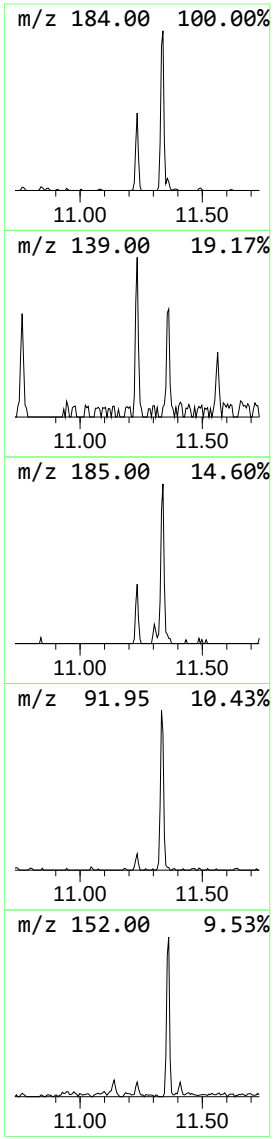
****

Peak Number 4 Naphtho[2,1-b]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.233	2.09 ng	125399	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	97
2	Dibenzothiophene	184	C12H8S	000132-65-0	96
3	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	93
4	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	93
5	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

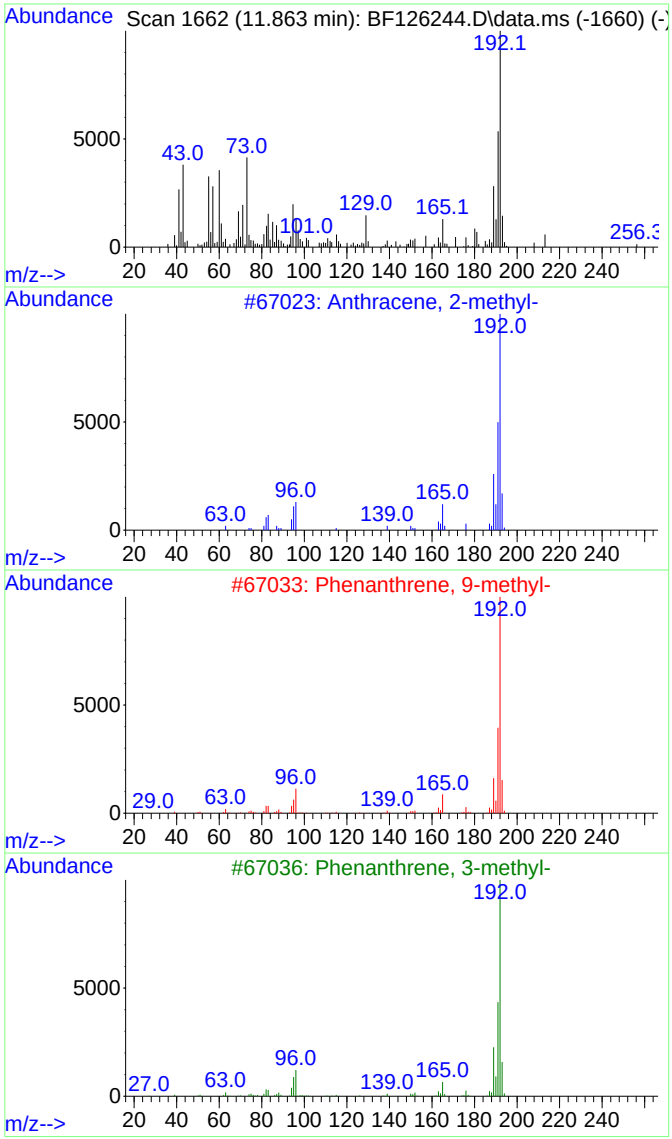
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

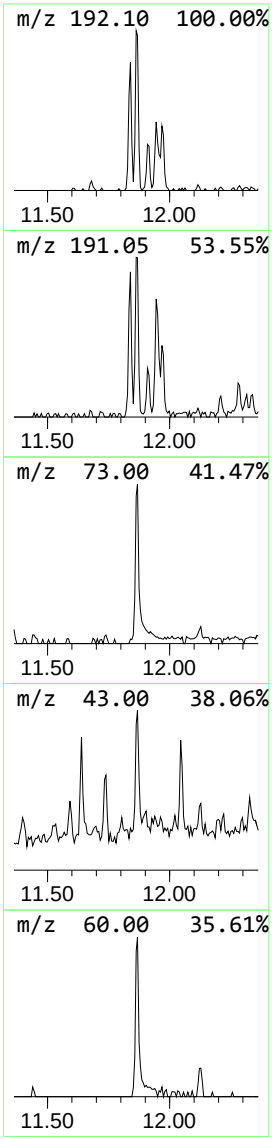
****

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.42 ng	205630	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	92
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	92
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

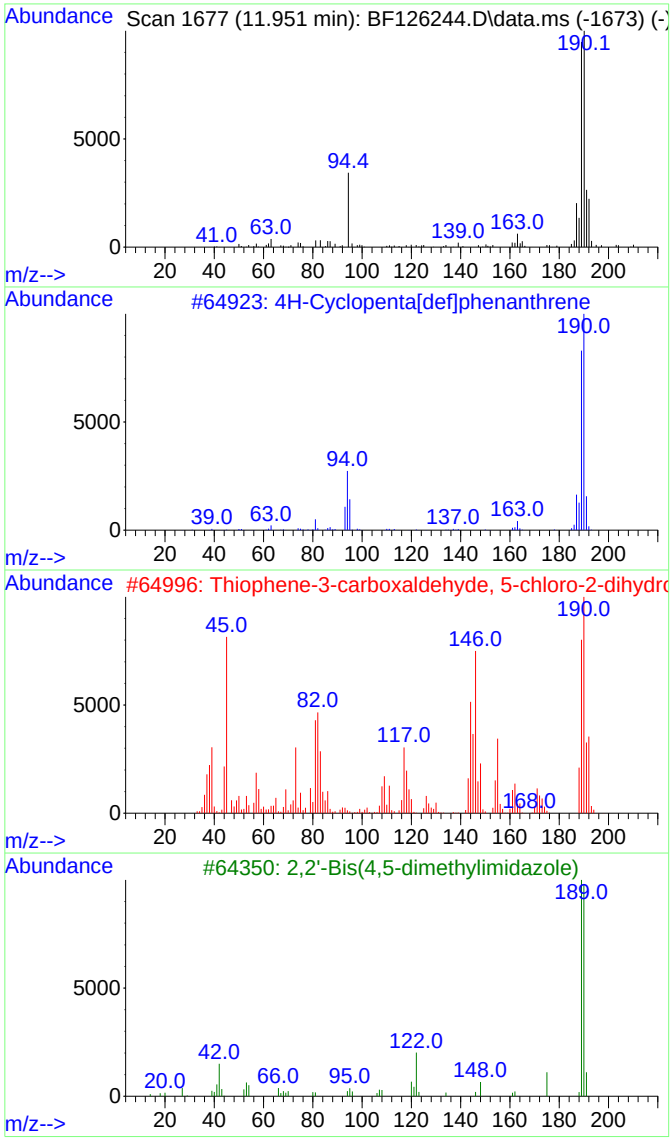
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

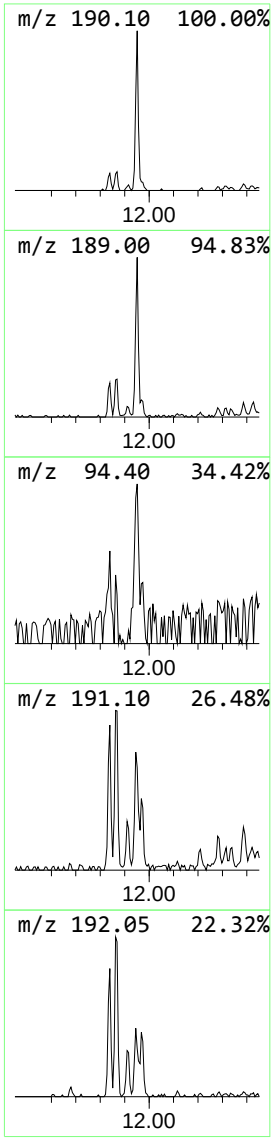
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.29 ng	137950	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	36
5	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

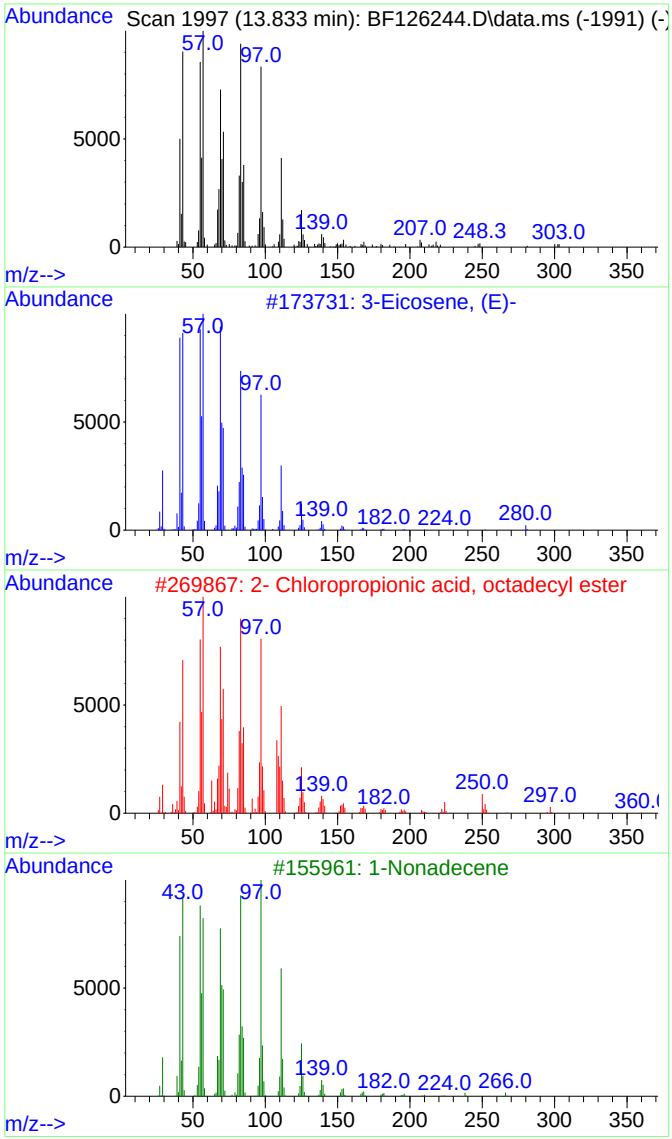
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

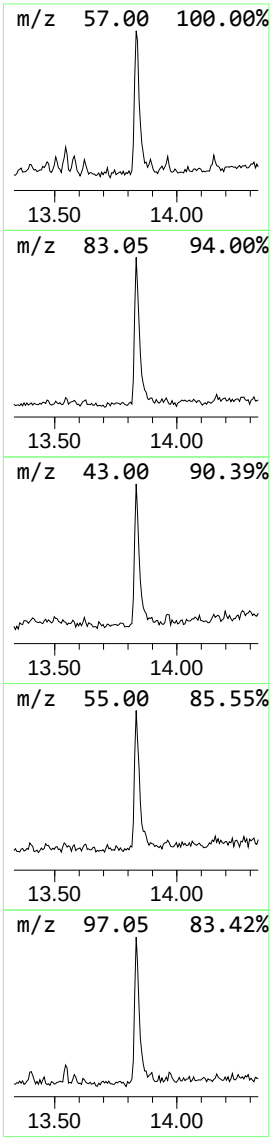
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	6.45 ng	418721	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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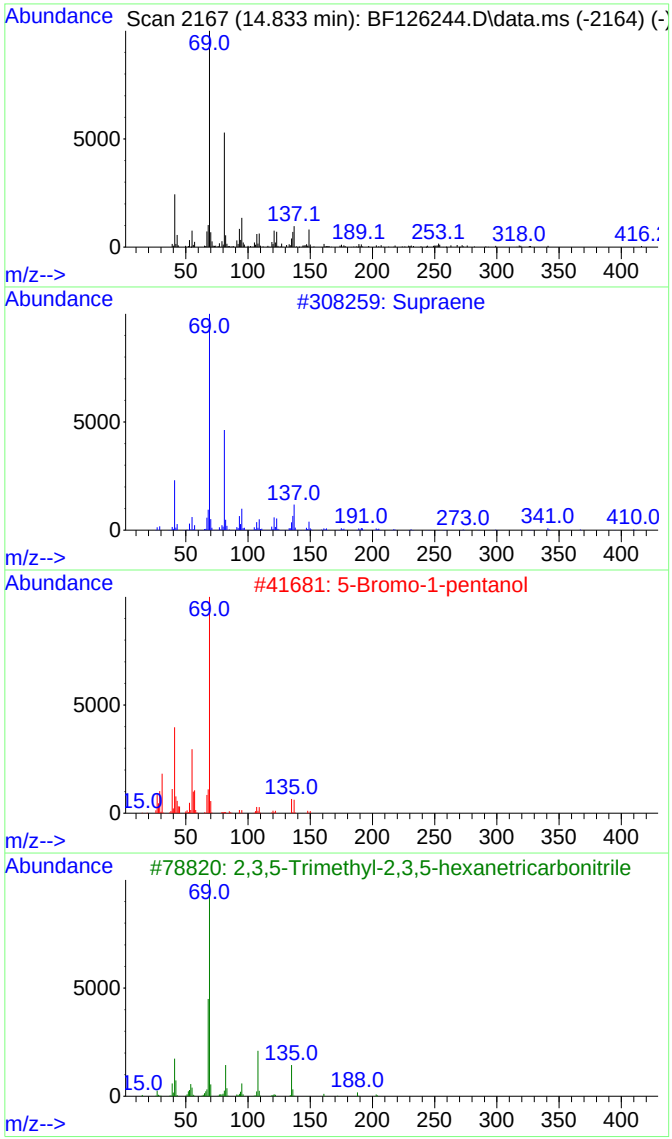
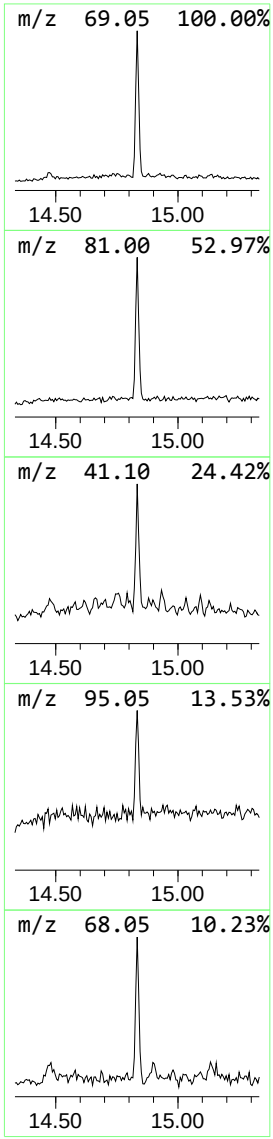
Peak Number 8 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	6.84 ng	253001	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	53
3	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
4	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47
5	1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	067682-47-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126244.D
Acq On : 17 Dec 2021 20:03
Operator : JU/CG
Sample : M5078-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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
2-Pentanone, 4-...	5.028	11.7	ng	717251	1	6.816	1231790	20.0
Ethanol, 2-(2-b...	8.004	3.0	ng	233816	2	8.098	1568530	20.0
3-(2-Hydroxyeth...	9.304	3.8	ng	267829	3	9.857	1407760	20.0
Naphtho[2,1-b]t...	11.233	2.1	ng	125399	4	11.339	1202310	20.0
Anthracene, 2-m...	11.863	3.4	ng	205630	4	11.339	1202310	20.0
4H-Cyclopenta[d...	11.951	2.3	ng	137950	4	11.339	1202310	20.0
3-Eicosene, (E)-	13.833	6.5	ng	418721	5	13.974	1298160	20.0
Supraene	14.833	6.8	ng	253001	6	15.421	739466	20.0