LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139969.D
Acq On : 23 Oct 2024 17:30
Operator : RC/JU
Sample : P4458-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
280517

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	13	24	rVB	1044423	1630183	100.00%	8.173%
2	3.987	316	322	327	rVB	10747	16939	1.04%	0.085%
3	4.493	401	408	415	rBV	153591	217802	13.36%	1.092%
4	4.763	434	454	463	rVB3	6663	28785	1.77%	0.144%
5	5.098	505	511	521	rVB	126800	181560	11.14%	0.910%
6	5.498	573	579	584	rBV	1114026	1415038	86.80%	7.094%
7	6.504	744	750	758	rBV	1046483	1381440	84.74%	6.926%
8	6.887	810	815	821	rVB	788563	992710	60.90%	4.977%
9	7.163	856	862	866	rBV	12814	18161	1.11%	0.091%
10	7.445	904	910	915	rBV	691298	853017	52.33%	4.277%
11	7.698	949	953	958	rBV	27916	35017	2.15%	0.176%
12	8.169	1028	1033	1038	rBV	973466	1205101	73.92%	6.042%
13	8.381	1064	1069	1077	rVB2	23183	34064	2.09%	0.171%
14	8.710	1122	1125	1129	rVV	26667	37353	2.29%	0.187%
15	9.163	1199	1202	1205	rBV	15197	20401	1.25%	0.102%
16	9.245	1210	1216	1226	rBV	1076719	1416999	86.92%	7.104%
17	9.328	1226	1230	1237	rVB5	18314	31728	1.95%	0.159%
18	9.575	1263	1272	1275	rBV7	7565	18049	1.11%	0.090%
19	9.645	1280	1284	1288	rVB	15441	20158	1.24%	0.101%
20	9.798	1305	1310	1314	rBV2	21667	30935	1.90%	0.155%
21	9.922	1325	1331	1336	rBV	889299	1197970	73.49%	6.006%
22	10.086	1355	1359	1362	rBV3	20374	25670	1.57%	0.129%
23	10.128	1362	1366	1370	rVB	16611	23289	1.43%	0.117%
24	10.333	1396	1401	1407	rBV4	12762	18821	1.15%	0.094%
25	10.469	1420	1424	1430	rVB2	48028	61273	3.76%	0.307%
26	10.575	1437	1442	1447	rVB	18564	28476	1.75%	0.143%
27	10.633	1448	1452	1457	rVB	72561	87756	5.38%	0.440%
28	10.710	1460	1465	1471	rBV	555944	733600	45.00%	3.678%
29	10.763	1471	1474	1478	rVB2	21907	24973	1.53%	0.125%
30	10.839	1483	1487	1495	rVB	67882	95224	5.84%	0.477%
31	10.916	1496	1500	1508	rBV6	13695	26498	1.63%	0.133%
32	11.039	1517	1521	1525	rBV2	30246	45563	2.79%	0.228%
33	11.304	1562	1566	1570	rVB	49093	63970	3.92%	0.321%
34	11.410	1579	1584	1592	rBV2	828384	1191446	73.09%	5.973%
35	11.486	1592	1597	1600	rVV	38960	65224	4.00%	0.327%
36	11.522	1600	1603	1612	rVB4	18703	39893	2.45%	0.200%

LSC Area Percent Report

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Sample : P4458-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.657	1619	1626	1630	rBV4	14295	32931	2.02%	0.165%
38	11.751	1638	1642	1648	rVB	29316	44396	2.72%	0.223%
39	11.892	1660	1666	1667	rBV5	26128	41159	2.52%	0.206%
40	11.933	1668	1673	1678	rVB3	123687	186979	11.47%	0.937%
41	12.021	1684	1688	1696	rVB3	41711	82678	5.07%	0.415%
42	12.392	1748	1751	1757	rVB5	11187	17453	1.07%	0.087%
43	12.498	1765	1769	1774	rVB2	39539	52295	3.21%	0.262%
44	12.621	1785	1790	1795	rBV	184795	238674	14.64%	1.197%
45	12.716	1803	1806	1811	rBV	39024	63847	3.92%	0.320%
46	12.851	1820	1829	1835	rBV	164991	288212	17.68%	1.445%
47	12.992	1848	1853	1862	rVB	935637	1241703	76.17%	6.225%
48	13.068	1862	1866	1870	rBV3	17855	32532	2.00%	0.163%
49	13.180	1882	1885	1888	rVB	31383	36794	2.26%	0.184%
50	13.245	1893	1896	1899	rVV	22267	29934	1.84%	0.150%
51	13.904	2004	2008	2014	rVB3	46279	74626	4.58%	0.374%
52	14.051	2027	2033	2044	rVB2	843346	1299853	79.74%	6.517%
53	14.680	2136	2140	2145	rVB	91103	122940	7.54%	0.616%
54	15.098	2207	2211	2219	rVB2	100476	218814	13.42%	1.097%
55	15.462	2270	2273	2279	rBV	52127	103115	6.33%	0.517%
56	15.527	2279	2284	2296	rVB	626305	1100573	67.51%	5.518%
57	15.686	2306	2311	2318	rVB	162417	272024	16.69%	1.364%
58	16.074	2374	2377	2387	rVB2	71571	133893	8.21%	0.671%
59	16.262	2404	2409	2421	rVB2	175725	368891	22.63%	1.849%
60	16.709	2479	2485	2497	rVB	202372	438208	26.88%	2.197%
61	16.956	2522	2527	2532	rVB2	58156	108774	6.67%	0.545%

Sum of corrected areas: 19946384

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Misc :
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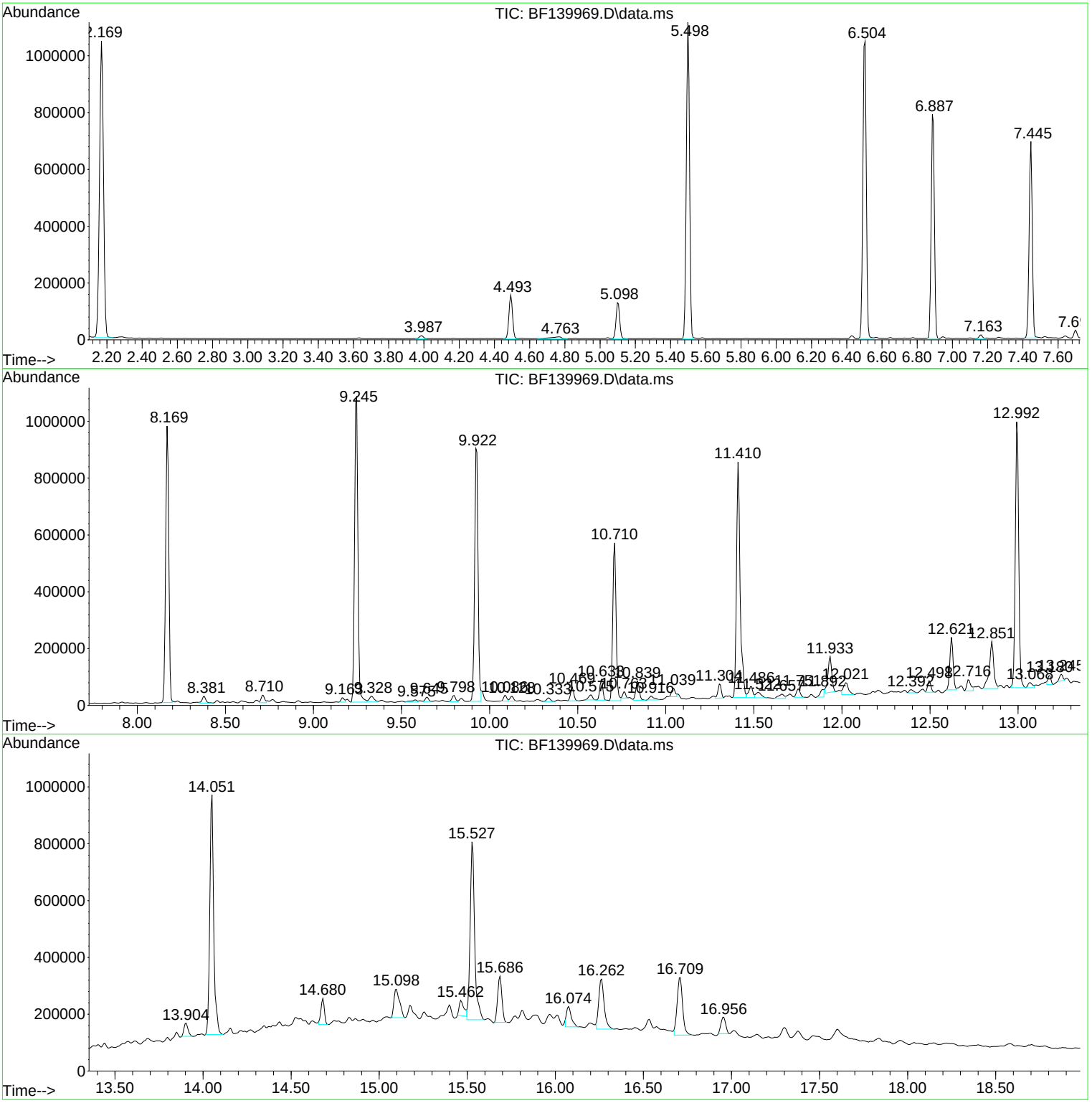
Instrument :
BNA_F
ClientSampleId :
280517

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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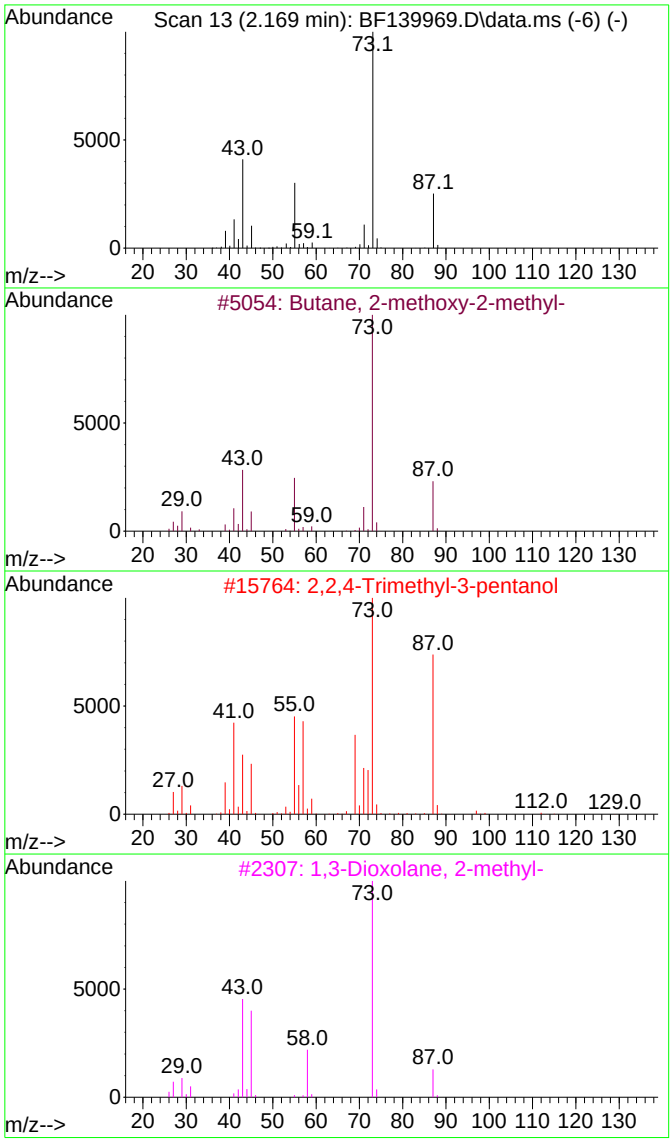
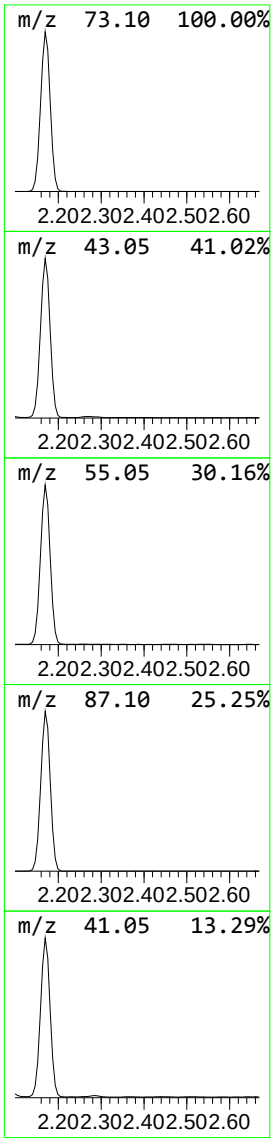
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	32.84 ng	1630180	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF139969.D
Acq On : 23 Oct 2024 17:30
Operator : RC/JU
Sample : P4458-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

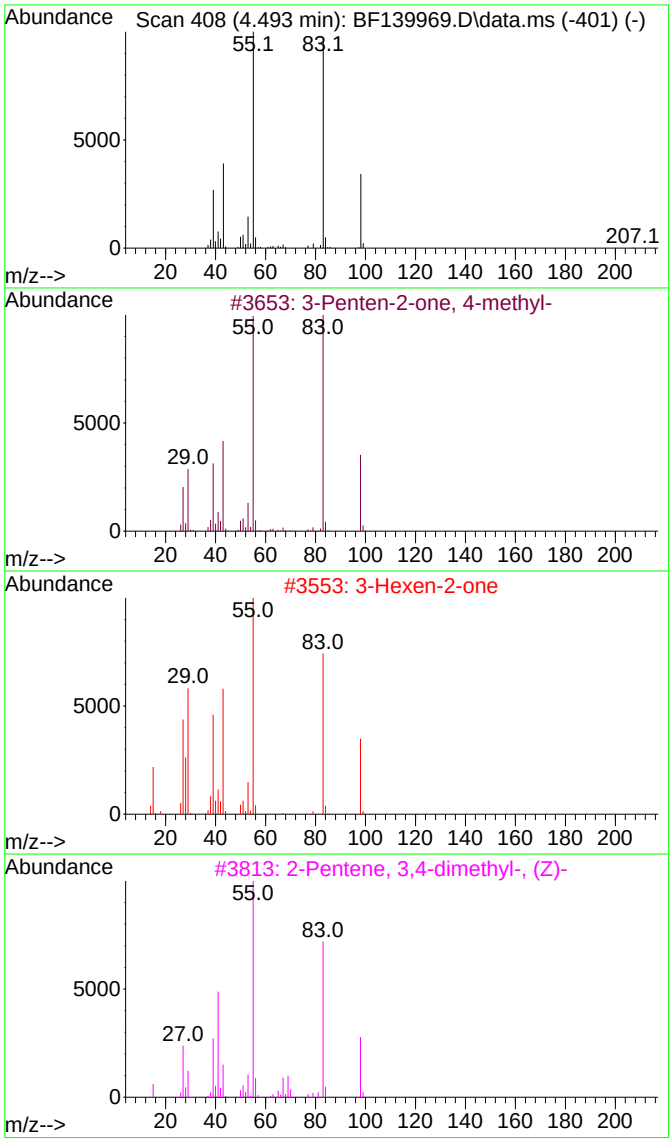
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

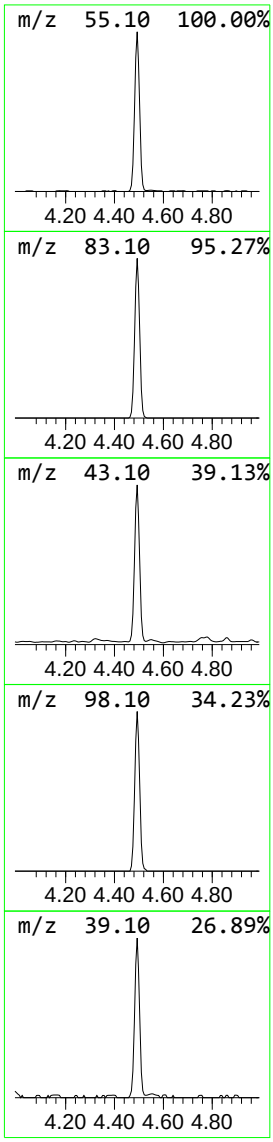
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.493	4.39 ng	217802	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86





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Sample : P4458-01 2X
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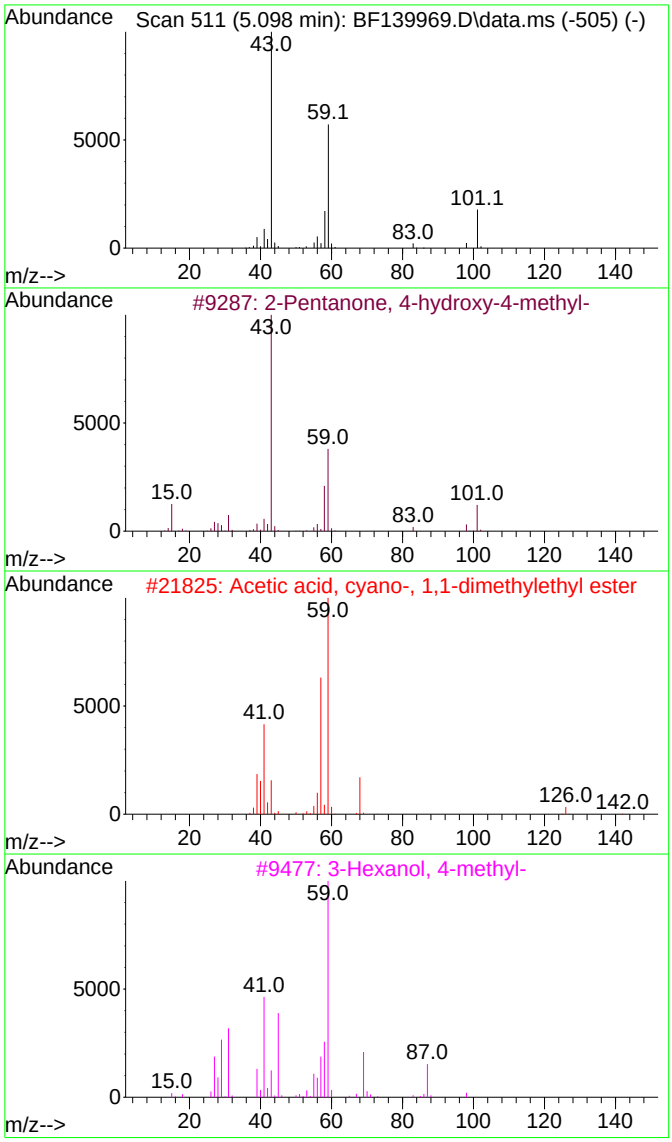
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

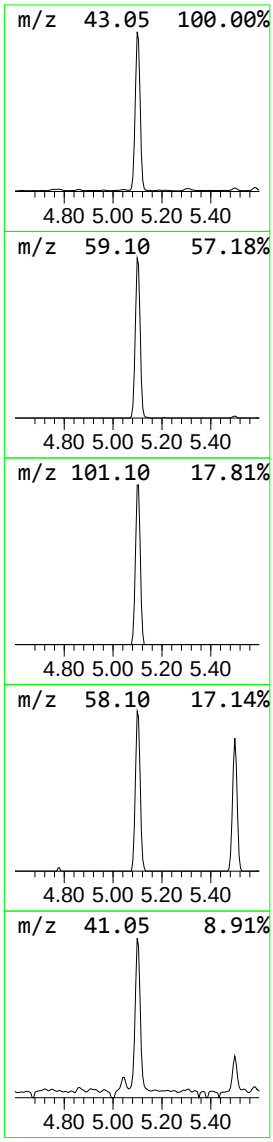
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.66 ng	181560	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

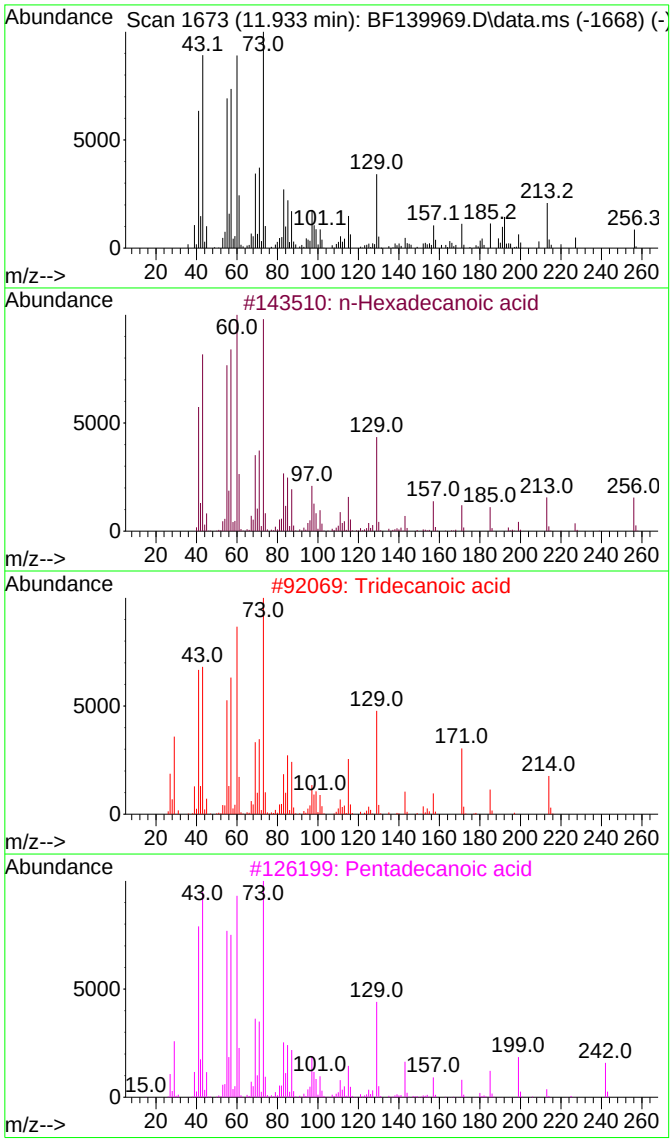
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

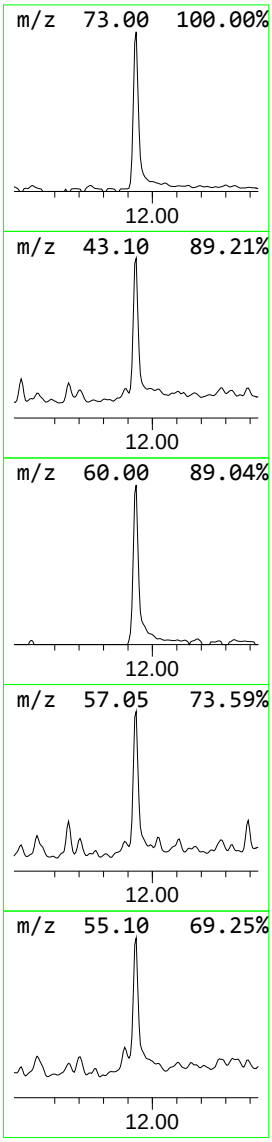
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.14 ng	186979	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Octanoic acid	144	C8H16O2	000124-07-2	60





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

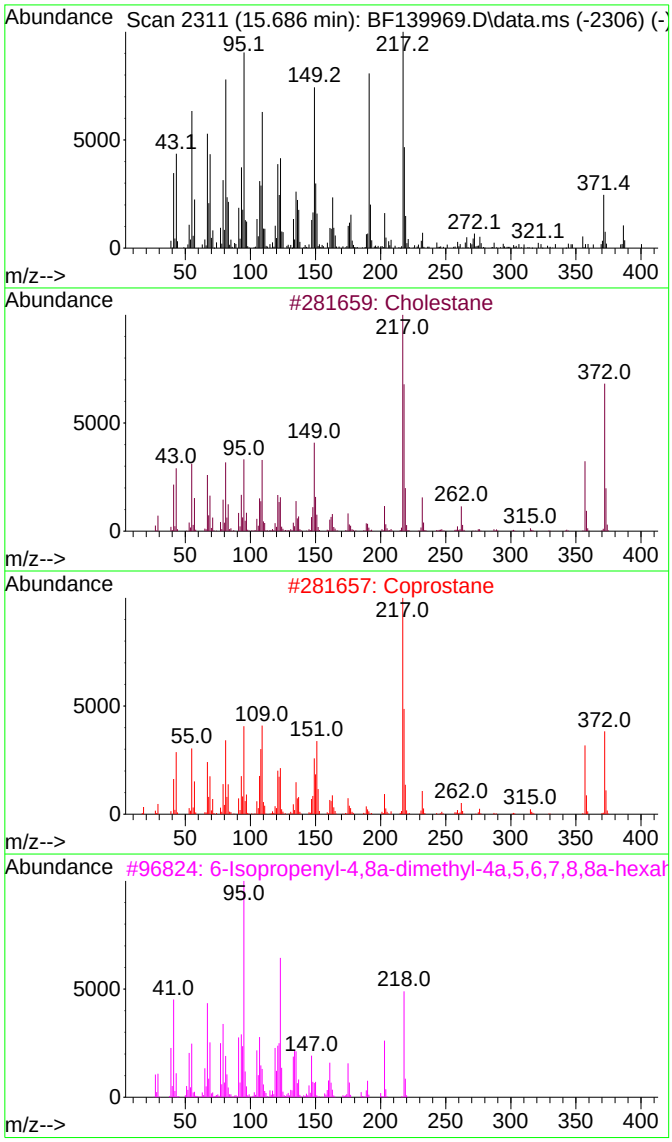
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

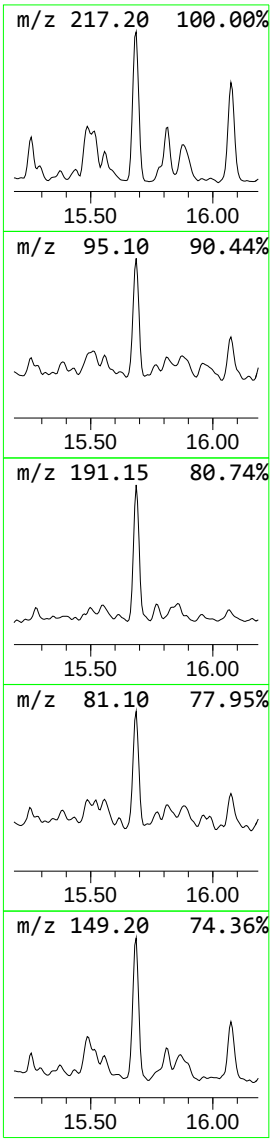
****

Peak Number 5 Cholestane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.686	4.94 ng	272024	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestane	372	C27H48	000481-21-0	78
2	Coprostane	372	C27H48	000481-20-9	52
3	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	49
4	(1R,2S,8R,8Ar)-8-acetoxy-1-(2-hy...	296	C18H32O3	1000298-98-4	40
5	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

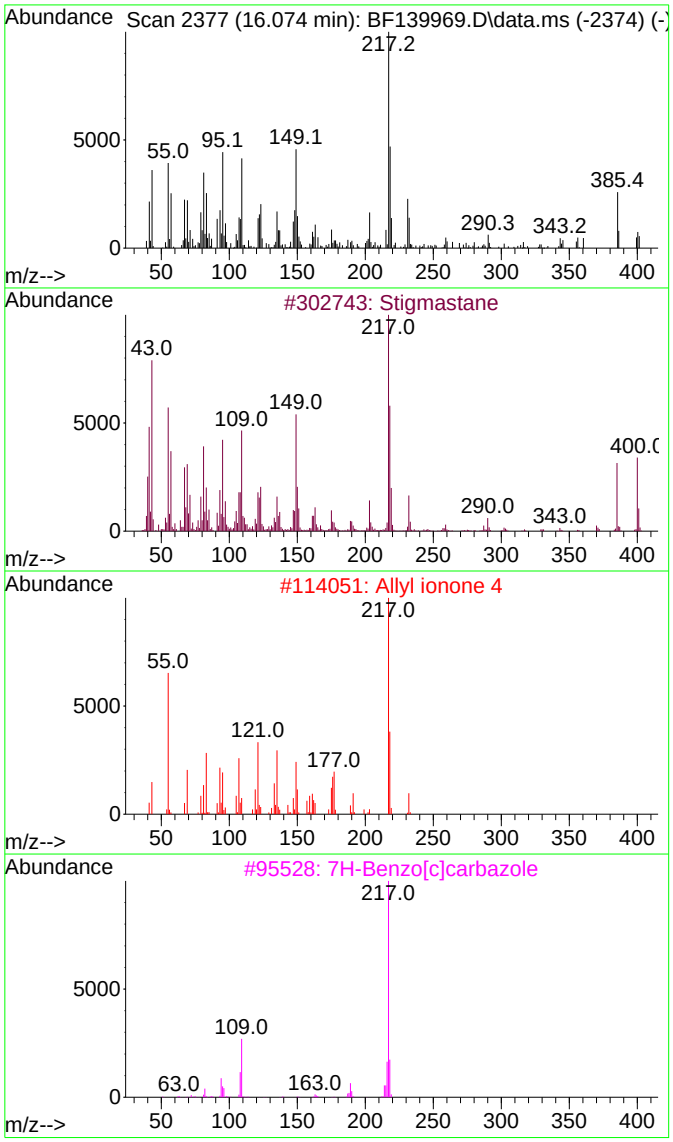
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

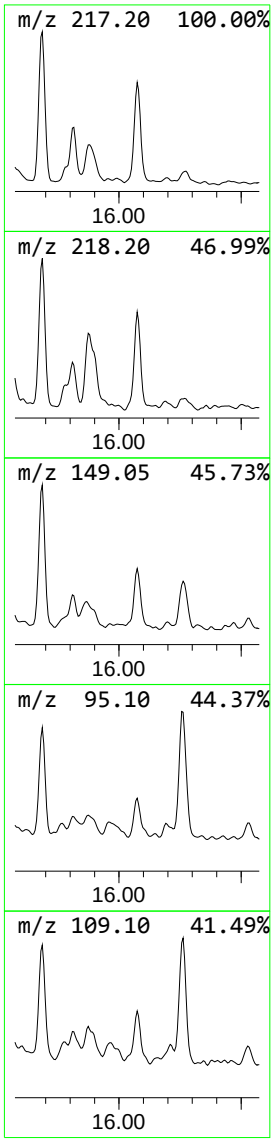
****

Peak Number 6 Stigmastane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.074	2.43 ng	133893	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmastane	400	C29H52	000601-58-1	72
2	Allyl ionone 4	232	C16H24O	1000284-93-0	38
3	7H-Benzo[c]carbazole	217	C16H11N	000205-25-4	22
4	11H-Benzo[a]carbazole	217	C16H11N	000239-01-0	22
5	p-Octylacetophenone	232	C16H24O	010541-56-7	14





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Data File : BF139969.D
Acq On : 23 Oct 2024 17:30
Operator : RC/JU
Sample : P4458-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
280517

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

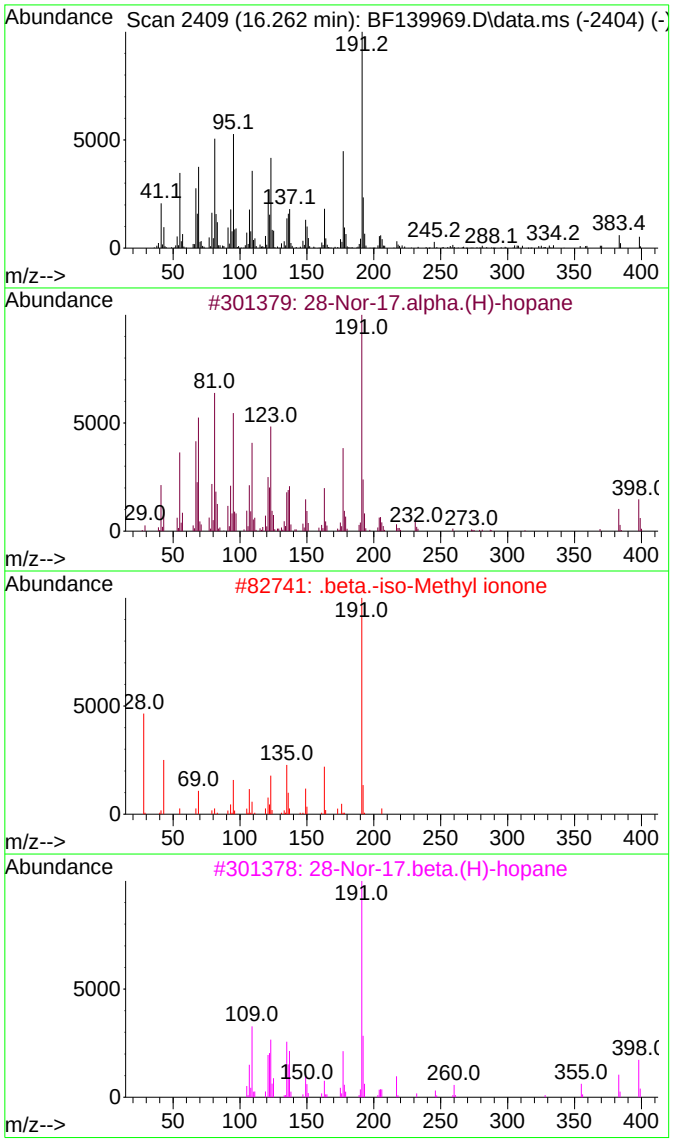
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

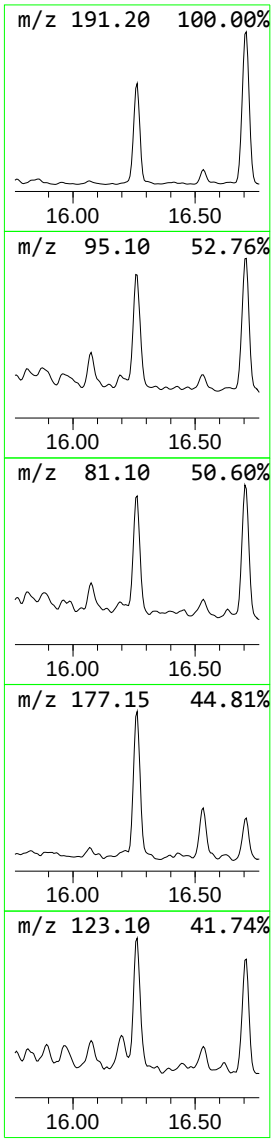
****

Peak Number 7 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	6.70 ng	368891	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	96
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	62
3	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	58
4	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	47
5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	37





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Instrument :
BNA_F
ClientSampleId :
280517

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

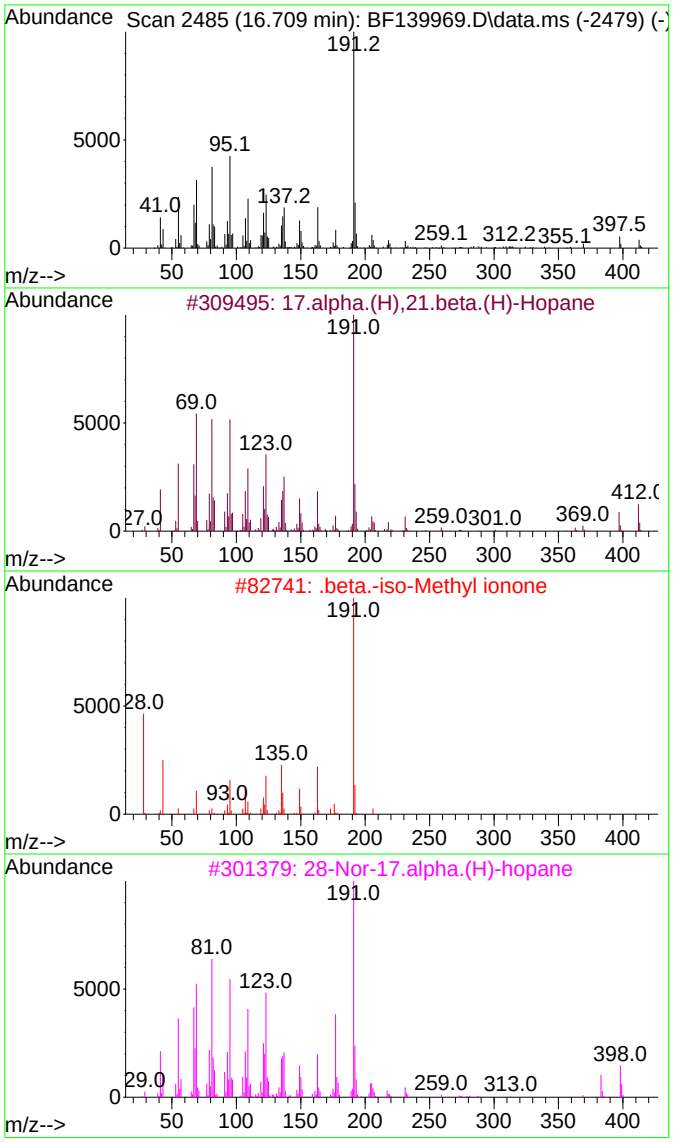
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

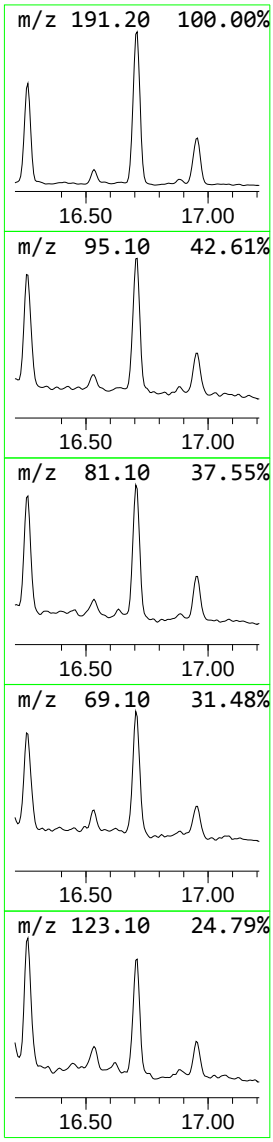
****

Peak Number 8 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.709	7.96 ng	438208	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	96
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	81
3	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	55
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	49
5	4-Fluoro-3-(trifluoromethyl)phen...	284	C9H5BrF4O	537050-14-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139969.D
Acq On : 23 Oct 2024 17:30
Operator : RC/JU
Sample : P4458-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
280517

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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
Butane, 2-metho...	2.169	32.8	ng	1630180	1	6.887	992710	20.0
3-Penten-2-one,...	4.493	4.4	ng	217802	1	6.887	992710	20.0
2-Pentanone, 4-...	5.098	3.7	ng	181560	1	6.887	992710	20.0
n-Hexadecanoic ...	11.933	3.1	ng	186979	4	11.410	1191450	20.0
Cholestane	15.686	4.9	ng	272024	6	15.527	1100570	20.0
Stigmastane	16.074	2.4	ng	133893	6	15.527	1100570	20.0
28-Nor-17.alpha...	16.262	6.7	ng	368891	6	15.527	1100570	20.0
17.alpha.(H),21...	16.709	8.0	ng	438208	6	15.527	1100570	20.0