LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039399.D
Acq On : 11 Apr 2023 18:37
Operator : CG/JU
Sample : 02262-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-1-040723

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_M\Methods\8270-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.952	295	300	310	rBV	535239	763451	12.05%	1.265%
2	5.428	374	381	399	rBV	1121958	1876286	29.62%	3.110%
3	6.387	540	544	550	rBV	41049	81605	1.29%	0.135%
4	7.040	648	655	673	rBV	1066763	1871430	29.54%	3.102%
5	7.863	786	795	806	rBV	798194	1326364	20.94%	2.199%
6	9.034	987	994	1011	rBV	644750	1173776	18.53%	1.946%
7	10.675	1262	1273	1280	rBV	1083965	1911394	30.17%	3.168%
8	10.851	1296	1303	1333	rBV	1146265	2171202	34.28%	3.599%
9	12.981	1661	1665	1673	rBV	31385	72667	1.15%	0.120%
10	13.139	1686	1692	1711	rBV	1881467	2846698	44.94%	4.719%
11	14.069	1845	1850	1855	rBV2	62948	103056	1.63%	0.171%
12	14.239	1874	1879	1892	rVB	87808	156293	2.47%	0.259%
13	14.522	1920	1927	1933	rBV	1556024	2413124	38.09%	4.000%
14	14.580	1933	1937	1946	rVB	120253	198613	3.14%	0.329%
15	14.916	1989	1994	2003	rBV	61246	110491	1.74%	0.183%
16	15.569	2100	2105	2115	rVB	100664	177355	2.80%	0.294%
17	15.880	2151	2158	2163	rVB2	99001	176951	2.79%	0.293%
18	16.010	2174	2180	2190	rBV	1424838	2115397	33.39%	3.506%
19	16.245	2213	2220	2227	rBV4	66248	165606	2.61%	0.275%
20	16.674	2289	2293	2298	rBV3	44945	69116	1.09%	0.115%
21	16.804	2312	2315	2319	rBV3	62190	71173	1.12%	0.118%
22	16.927	2332	2336	2341	rBV	58568	91249	1.44%	0.151%
23	17.086	2360	2363	2370	rVB	78429	121253	1.91%	0.201%
24	17.269	2389	2394	2398	rBV	1846763	2750231	43.42%	4.559%
25	17.310	2398	2401	2411	rVV	1563262	2252140	35.55%	3.733%
26	17.404	2412	2417	2422	rVV	400473	559613	8.83%	0.928%
27	17.680	2461	2464	2473	rVB2	74744	129215	2.04%	0.214%
28	18.168	2539	2547	2550	rBV2	637511	1278754	20.19%	2.120%
29	18.280	2562	2566	2571	rBV	173684	260141	4.11%	0.431%
30	18.345	2572	2577	2581	rBV2	386534	708560	11.19%	1.175%
31	18.651	2626	2629	2633	rVB	167699	205315	3.24%	0.340%
32	18.698	2634	2637	2642	rVB	129741	173135	2.73%	0.287%
33	19.068	2696	2700	2706	rBV2	186893	391275	6.18%	0.649%
34	19.333	2740	2745	2751	rBV	3569728	4742773	74.87%	7.862%
35	19.451	2762	2765	2774	rVB2	296398	486979	7.69%	0.807%
36	19.698	2803	2807	2815	rVB	3356870	4692266	74.07%	7.778%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
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Operator : CG/JU
Sample : 02262-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-1-040723

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_M\Methods\8270-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.898	2836	2841	2846	rBV	2854606	3582631	56.56%	5.939%
38	21.145	3051	3053	3060	rBV3	528135	1050520	16.58%	1.741%
39	21.457	3101	3106	3111	rBV2	2918377	6334633	100.00%	10.500%
40	21.498	3111	3113	3121	rVB	1872981	2451599	38.70%	4.064%
41	23.127	3386	3390	3396	rBV	1327225	3161378	49.91%	5.240%
42	23.750	3492	3496	3503	rVB	1548769	2837776	44.80%	4.704%
43	23.856	3510	3514	3519	rVB2	1281579	2214881	34.96%	3.671%

Sum of corrected areas: 60328365

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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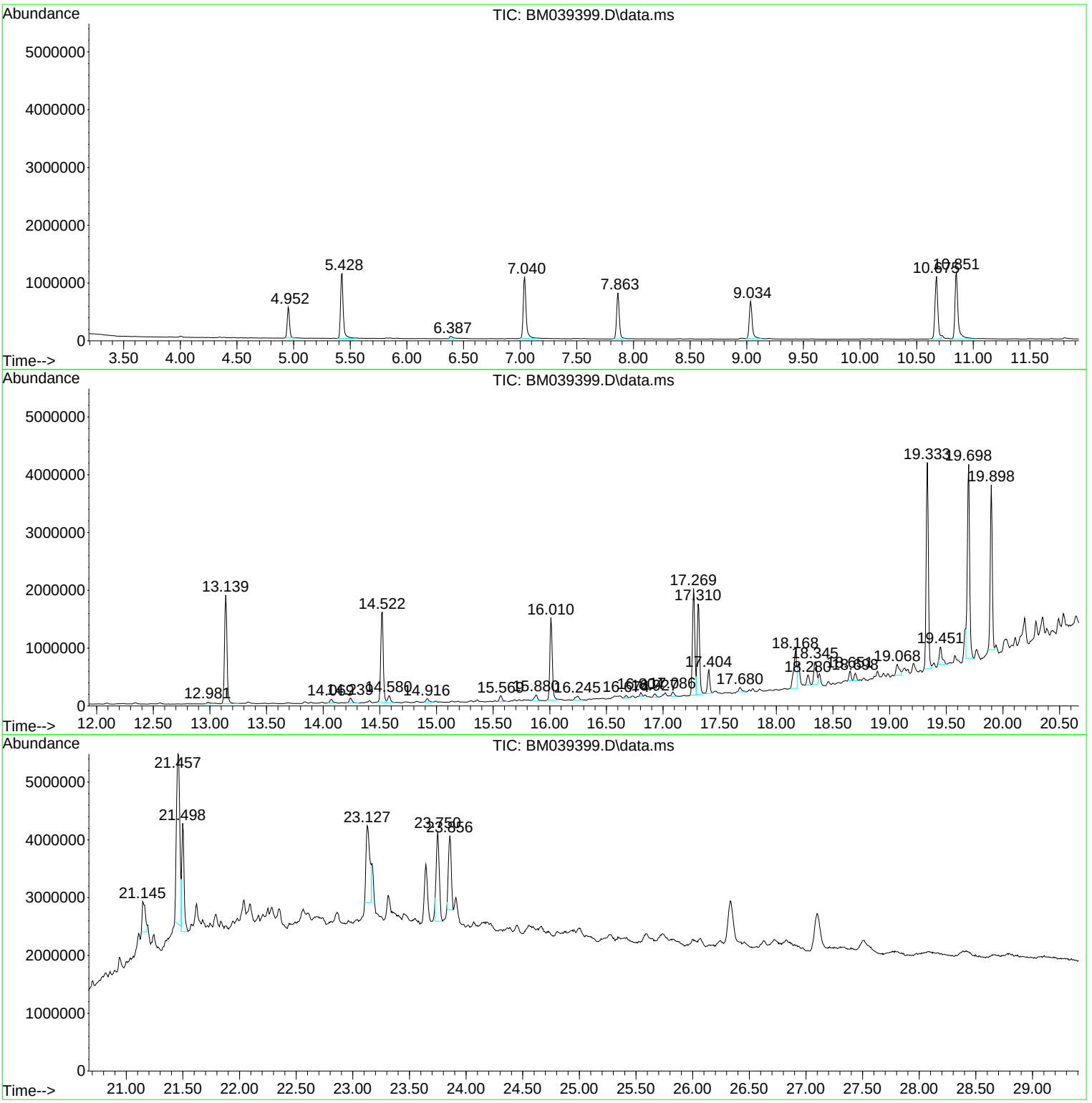
ClientSampleId :
JPP-1-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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_M\Data\BM041123\
Data File : BM039399.D
Acq On : 11 Apr 2023 18:37
Operator : CG/JU
Sample : 02262-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
JPP-1-040723

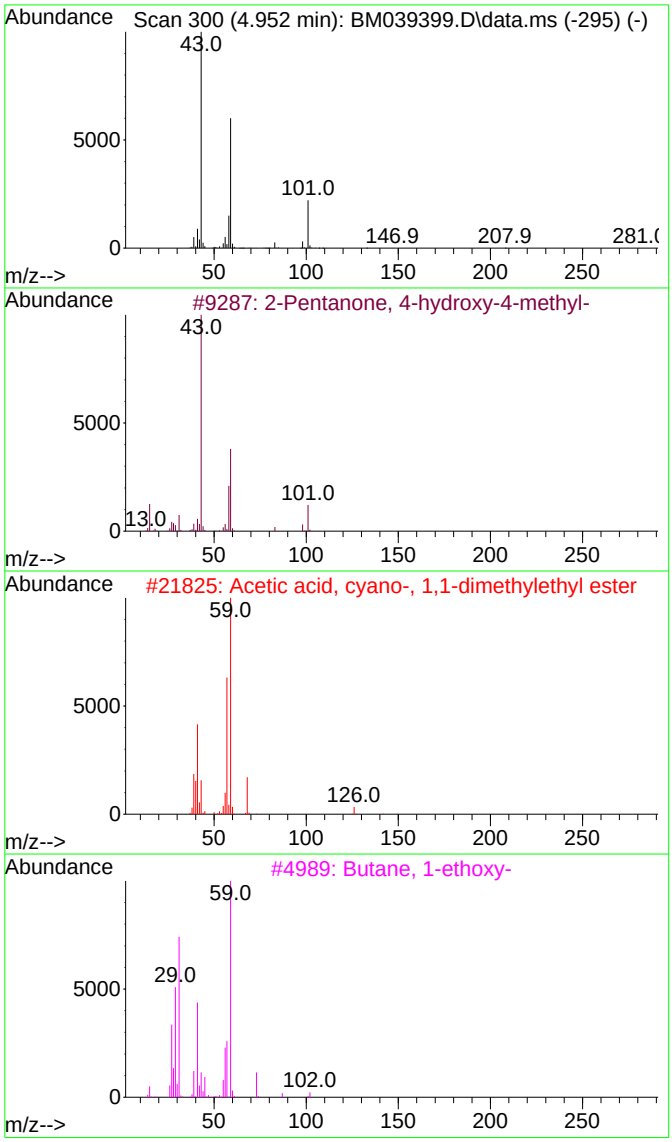
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

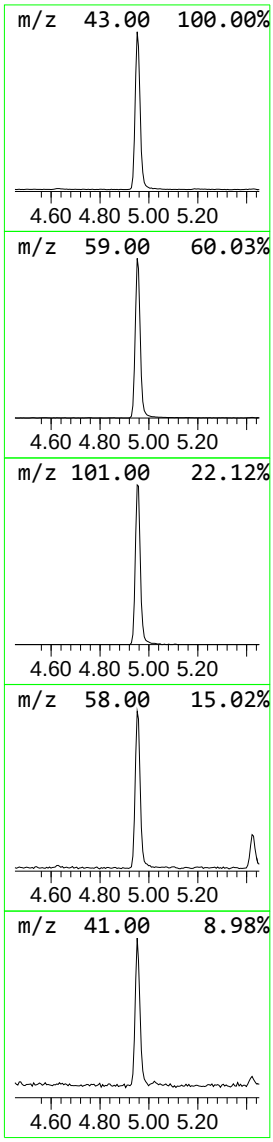
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.952	11.51 ng	763451	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BM039399.D
Acq On : 11 Apr 2023 18:37
Operator : CG/JU
Sample : 02262-07
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Instrument :
BNA_M
ClientSampleId :
JPP-1-040723

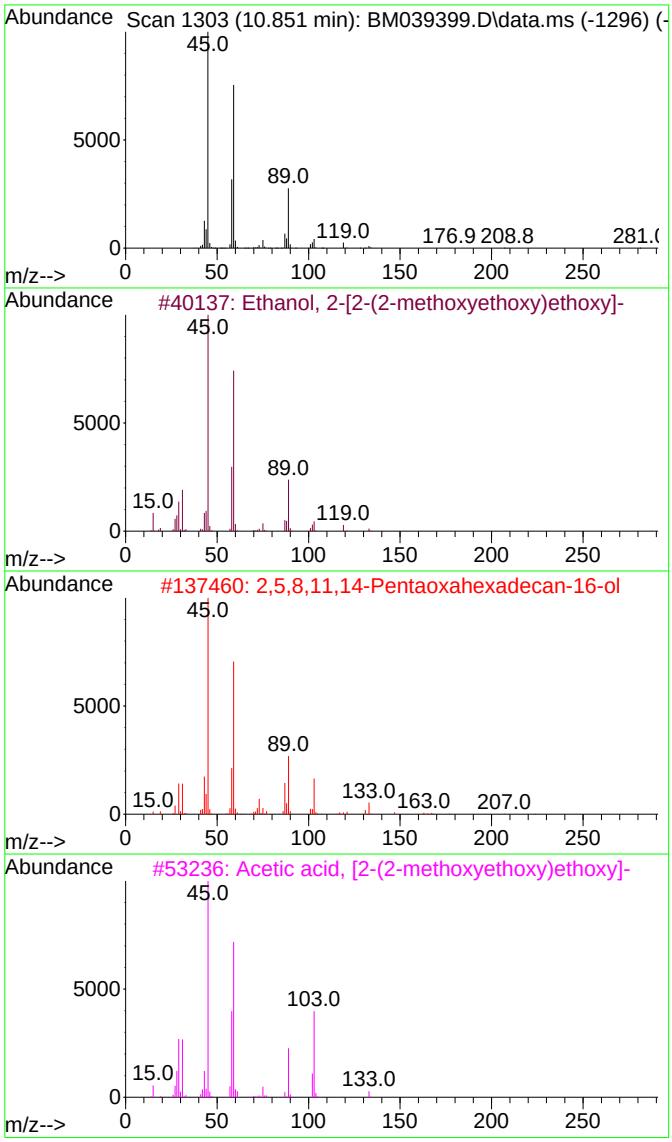
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

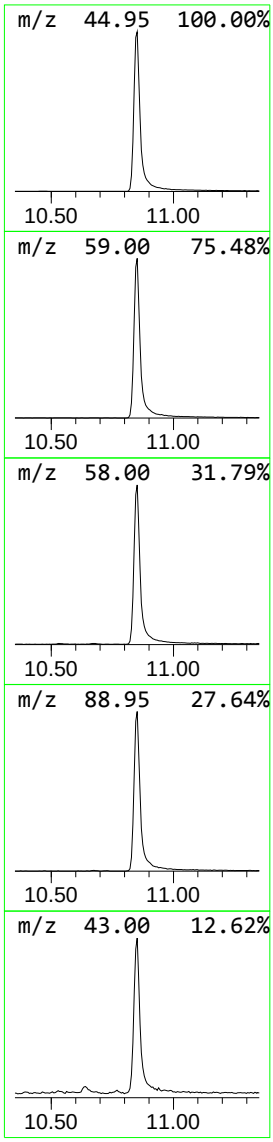
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-[2-(2-methoxyeth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	22.72 ng	2171200	Naphthalene-d8	10.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	90
2	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	72
3	Acetic acid, [2-(2-methoxyethoxy...	178	C7H14O5	016024-58-1	72
4	2-Propanol, 1,1'-oxybis-	134	C6H14O3	000110-98-5	64
5	Propane, 1,2,3-trimethoxy-	134	C6H14O3	020637-49-4	59





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Sample : 02262-07
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-1-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

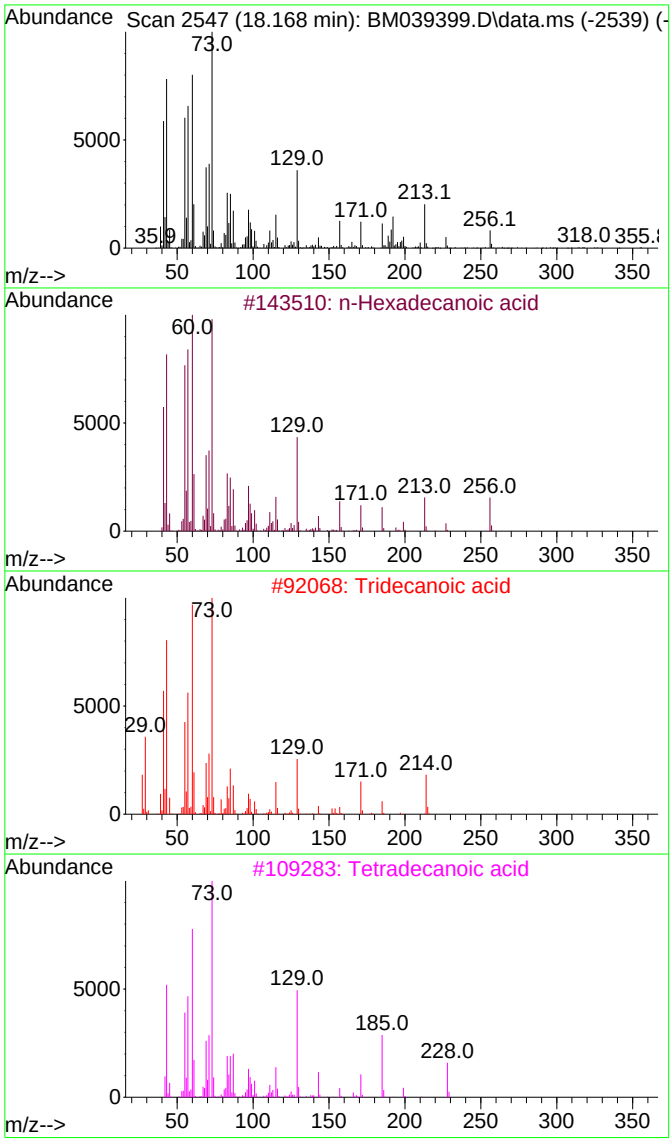
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

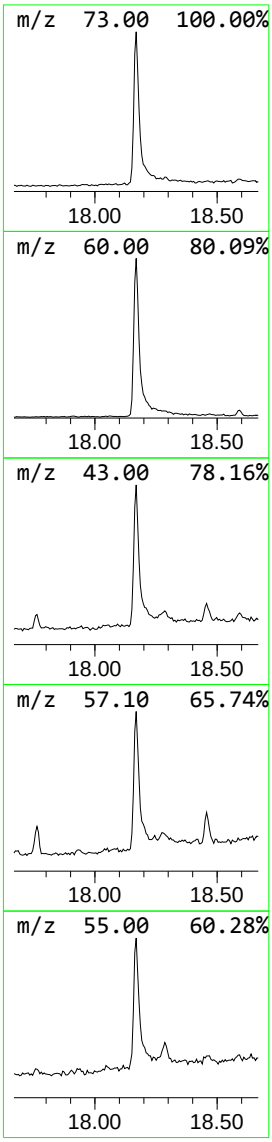
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	9.30 ng	1278750	Phenanthrene-d10	17.269

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039399.D
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Sample : 02262-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-1-040723

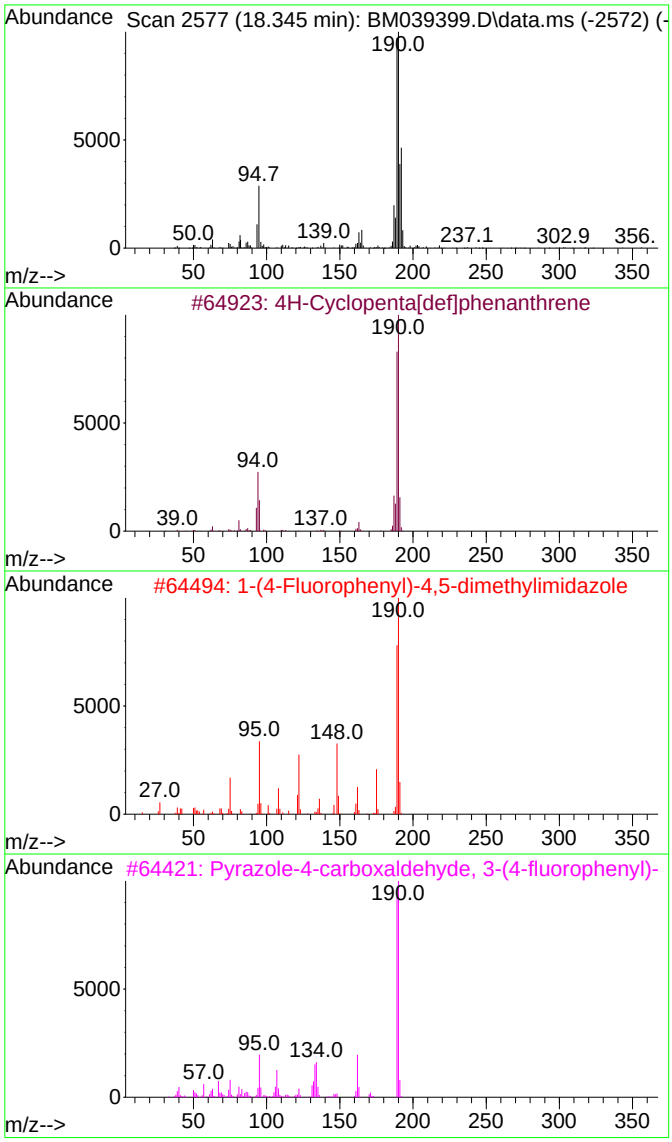
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

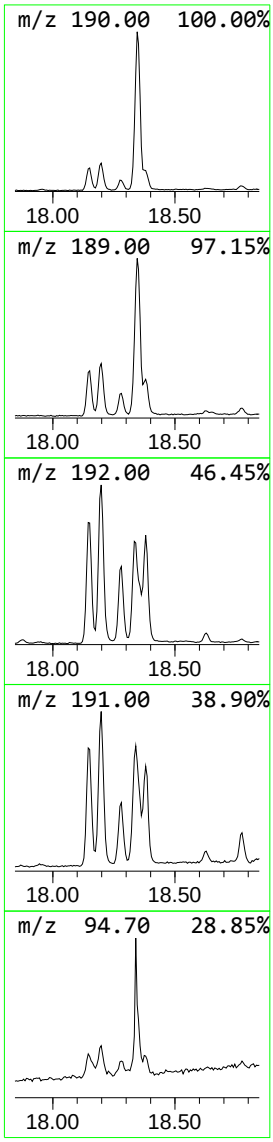
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	5.15 ng	708560	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2	1-(4-Fluorophenyl)-4,5-dimethyli...	190	C11H11FN2	1000443-18-7	50
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	Methyl diselenide	190	C2H6Se2	007101-31-7	38





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Sample : 02262-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
JPP-1-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

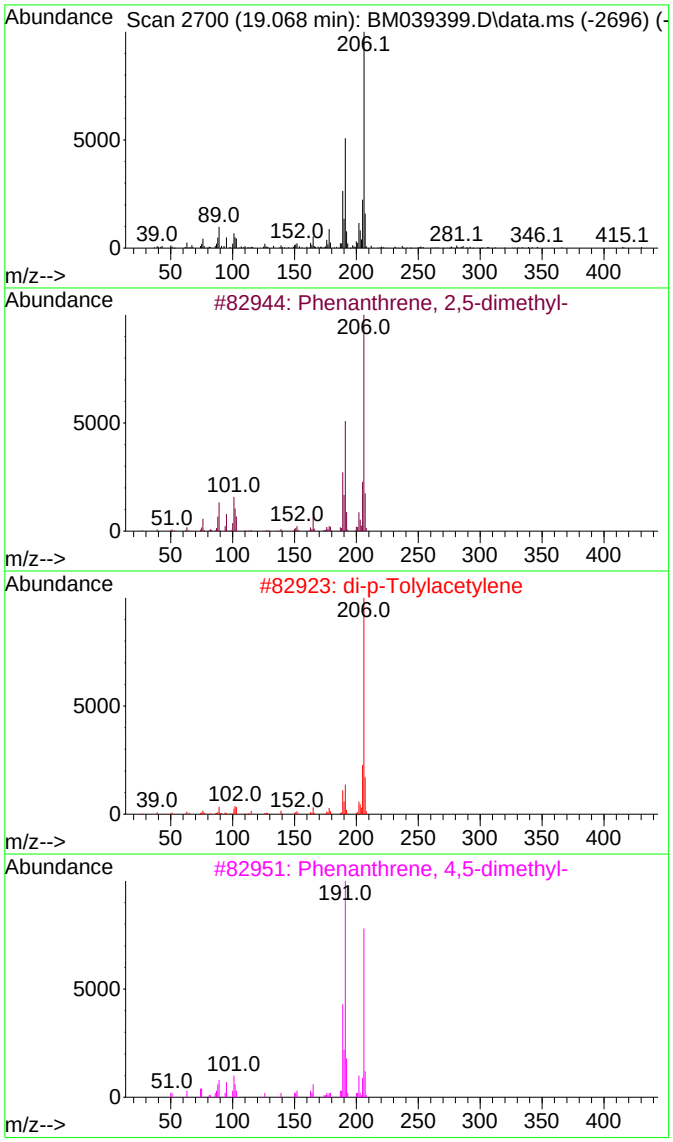
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

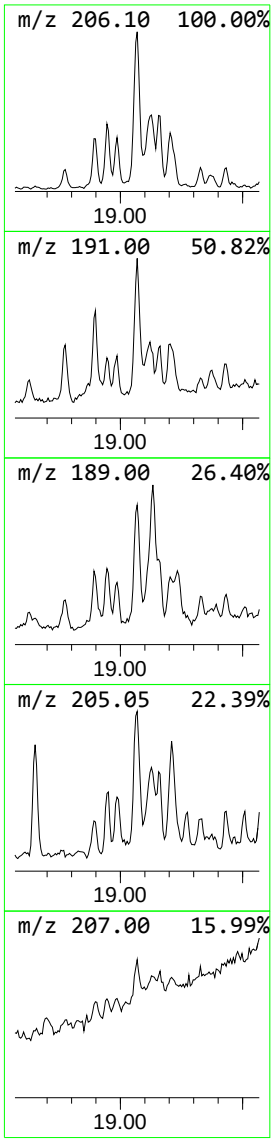
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.068	2.85 ng	391275	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	91
3	Phenanthrene, 4,5-dimethyl-	206	C16H14	003674-69-9	91
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	90
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

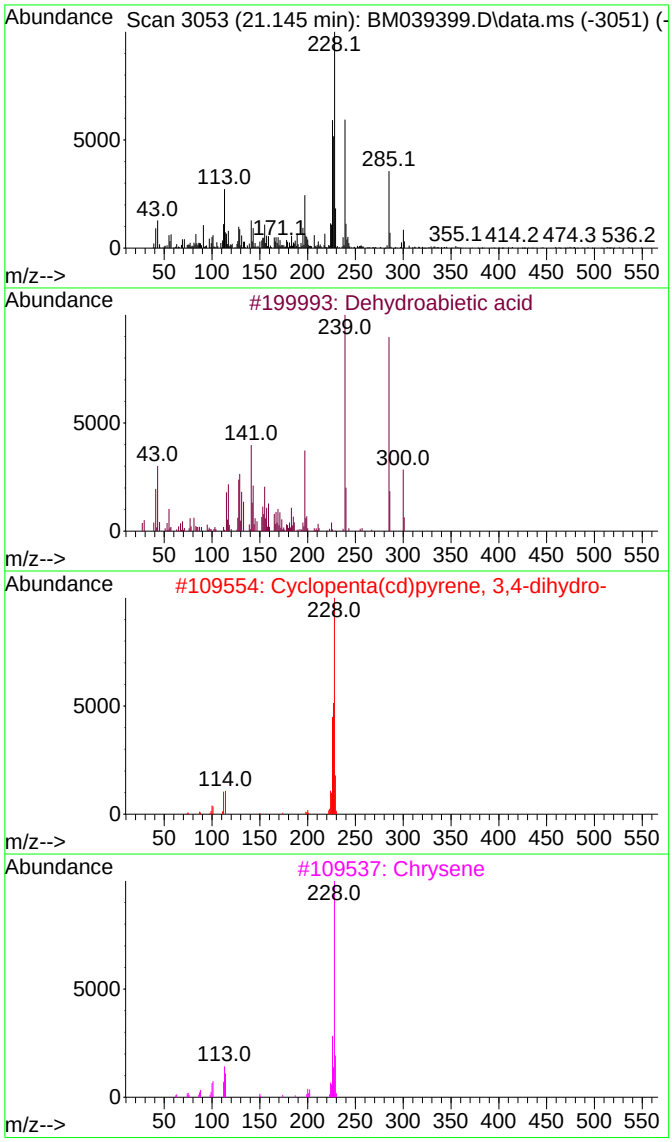
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

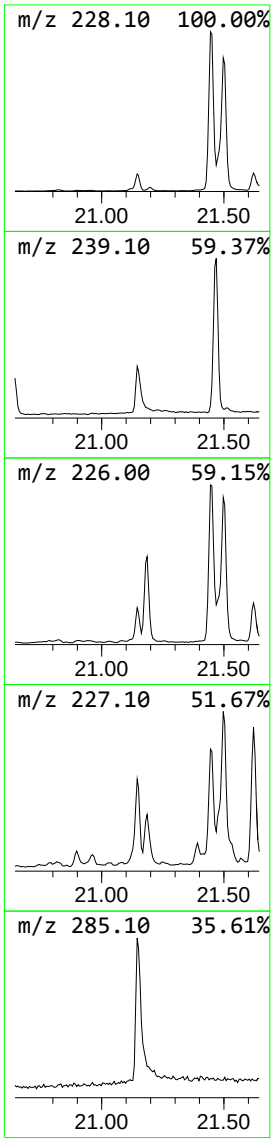
****

Peak Number 6 Dehydroabietic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	3.32 ng	1050520	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dehydroabietic acid	300	C20H28O2	001740-19-8	92
2	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	42
3	Chrysene	228	C18H12	000218-01-9	38
4	Triphenylene	228	C18H12	000217-59-4	38
5	5-Phenylthieno[2,3-d]pyrimidin-4-ol	228	C12H8N2OS	035978-39-3	30





Tentatively Identified Compound (LSC) summary

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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-...	4.952	11.5	ng	763451	1	7.863	1326360	20.0
Ethanol, 2-[2-(...	10.851	22.7	ng	2171200	2	10.675	1911390	20.0
n-Hexadecanoic ...	18.169	9.3	ng	1278750	4	17.269	2750230	20.0
4H-Cyclopenta[d...	18.345	5.2	ng	708560	4	17.269	2750230	20.0
Phenanthrene, 2...	19.068	2.9	ng	391275	4	17.269	2750230	20.0
Dehydroabietic ...	21.145	3.3	ng	1050520	5	21.462	6334630	20.0