LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082324\
Data File : BM047335.D
Acq On : 23 Aug 2024 16:08
Operator : RC/JU
Sample : P3686-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DNB-47-COMPOSITE

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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047335.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.263	61	64	71	rBV	72140	114646	2.43%	0.205%
2	4.563	278	285	294	rBV	135417	204809	4.35%	0.366%
3	5.010	355	361	374	rBV	2145280	3096927	65.70%	5.529%
4	6.569	619	626	643	rBV	2009825	3224057	68.40%	5.755%
5	7.351	751	759	768	rBV	1039372	1620577	34.38%	2.893%
6	8.498	947	954	964	rBV	1288326	2131867	45.23%	3.806%
7	9.086	1048	1054	1060	rBV	41247	76157	1.62%	0.136%
8	10.104	1219	1227	1232	rBV	1266858	2130694	45.20%	3.804%
9	10.151	1232	1235	1244	rVB	138521	233767	4.96%	0.417%
10	10.869	1351	1357	1369	rBV	73178	168032	3.56%	0.300%
11	11.780	1505	1512	1521	rBV	59711	100695	2.14%	0.180%
12	12.010	1545	1551	1558	rVB	43012	76381	1.62%	0.136%
13	12.616	1647	1654	1673	rBV	2690620	4046657	85.85%	7.224%
14	12.833	1685	1691	1698	rVB2	33282	67016	1.42%	0.120%
15	13.321	1767	1774	1780	rBV2	33542	67334	1.43%	0.120%
16	13.380	1780	1784	1793	rVB2	26116	48772	1.03%	0.087%
17	13.727	1831	1843	1850	rBV	84632	162528	3.45%	0.290%
18	14.010	1884	1891	1898	rBV	1883744	2820136	59.83%	5.034%
19	14.074	1898	1902	1912	rVB	196286	308326	6.54%	0.550%
20	14.245	1925	1931	1932	rBV4	65208	83337	1.77%	0.149%
21	14.421	1953	1961	1970	rBV	139264	235946	5.01%	0.421%
22	15.074	2066	2072	2084	rBV2	259704	408408	8.66%	0.729%
23	15.374	2118	2123	2135	rVB	47036	85345	1.81%	0.152%
24	15.521	2140	2148	2159	rBV	2566539	3895561	82.65%	6.954%
25	15.768	2185	2190	2198	rVB	24214	54687	1.16%	0.098%
26	16.086	2238	2244	2248	rBV3	37539	61136	1.30%	0.109%
27	16.439	2300	2304	2311	rVB2	40708	66110	1.40%	0.118%
28	16.515	2313	2317	2322	rBV3	31958	67161	1.42%	0.120%
29	16.592	2322	2330	2340	rVB	111229	220435	4.68%	0.394%
30	16.774	2355	2361	2365	rBV	2225426	3239325	68.73%	5.783%
31	16.815	2365	2368	2376	rVV	1853561	2599638	55.15%	4.641%
32	16.909	2376	2384	2391	rVV	434378	692534	14.69%	1.236%
33	16.980	2392	2396	2401	rVB2	39954	69190	1.47%	0.124%
34	17.192	2424	2432	2444	rBV	175093	337198	7.15%	0.602%
35	17.303	2447	2451	2456	rVV3	46422	74395	1.58%	0.133%
36	17.356	2458	2460	2470	rVB4	24714	55896	1.19%	0.100%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082324\
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Acq On : 23 Aug 2024 16:08
Operator : RC/JU
Sample : P3686-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DNB-47-COMPOSITE

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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.492	2481	2483	2490	rVB4	41628	61993	1.32%	0.111%
38	17.656	2505	2511	2515	rBV	155145	231281	4.91%	0.413%
39	17.709	2515	2520	2528	rVV2	489186	812351	17.23%	1.450%
40	17.780	2529	2532	2537	rVV2	96265	170244	3.61%	0.304%
41	17.845	2538	2543	2547	rVV2	291904	495270	10.51%	0.884%
42	17.886	2547	2550	2559	rVB	113308	175943	3.73%	0.314%
43	18.162	2593	2597	2602	rBV	117721	152931	3.24%	0.273%
44	18.209	2602	2605	2611	rVB	53024	71227	1.51%	0.127%
45	18.592	2665	2670	2674	rBV	78672	131573	2.79%	0.235%
46	18.650	2677	2680	2683	rVB3	37247	51107	1.08%	0.091%
47	18.733	2690	2694	2702	rBV3	52243	88628	1.88%	0.158%
48	18.850	2709	2714	2720	rBV	2093498	2817381	59.77%	5.029%
49	19.009	2737	2741	2748	rBV	167627	268722	5.70%	0.480%
50	19.097	2753	2756	2761	rVB	62333	91395	1.94%	0.163%
51	19.221	2768	2777	2782	rBV	1708425	2663195	56.50%	4.754%
52	19.409	2806	2809	2810	rBV	78837	79186	1.68%	0.141%
53	19.439	2810	2814	2819	rVV	3728840	4713422	100.00%	8.414%
54	19.692	2853	2857	2859	rBV2	84659	127063	2.70%	0.227%
55	19.727	2860	2863	2868	rVB	221169	307780	6.53%	0.549%
56	19.827	2877	2880	2884	rBV	193991	241577	5.13%	0.431%
57	19.886	2884	2890	2893	rVV3	125833	266122	5.65%	0.475%
58	20.021	2911	2913	2917	rBV	60409	71740	1.52%	0.128%
59	20.068	2919	2921	2926	rVV	61423	80309	1.70%	0.143%
60	20.750	3034	3037	3041	rVB4	217240	263558	5.59%	0.470%
61	21.015	3075	3082	3086	rBV2	2089109	3751734	79.60%	6.697%
62	21.050	3086	3088	3098	rVB	613147	816991	17.33%	1.458%
63	22.868	3392	3397	3403	rBV	370583	888711	18.85%	1.586%
64	23.580	3513	3518	3529	rVB	365685	814342	17.28%	1.454%
65	23.703	3533	3539	3548	rBV	1070491	2365690	50.19%	4.223%

Sum of corrected areas: 56017146

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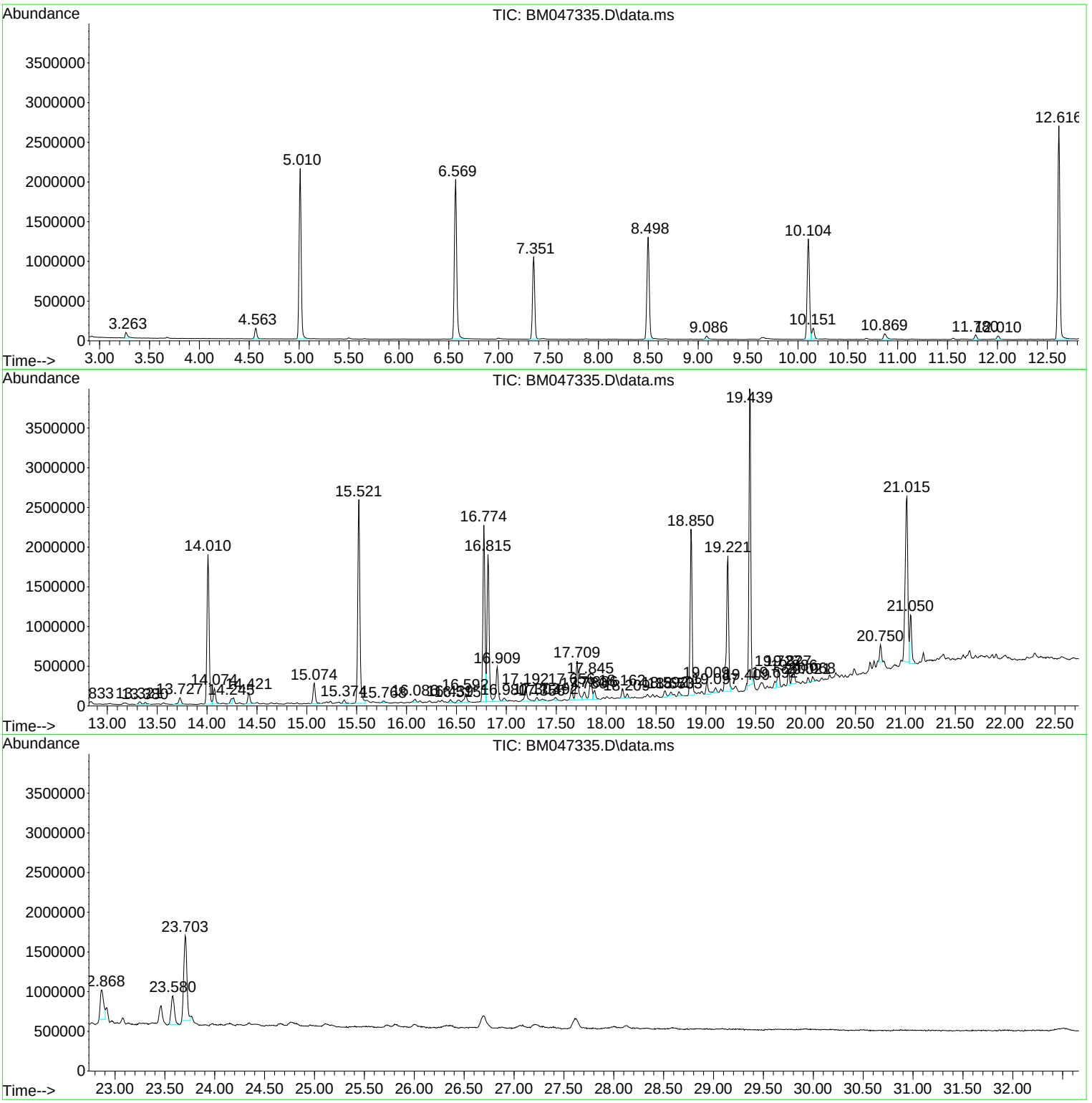
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DNB-47-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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Data File : BM047335.D
Acq On : 23 Aug 2024 16:08
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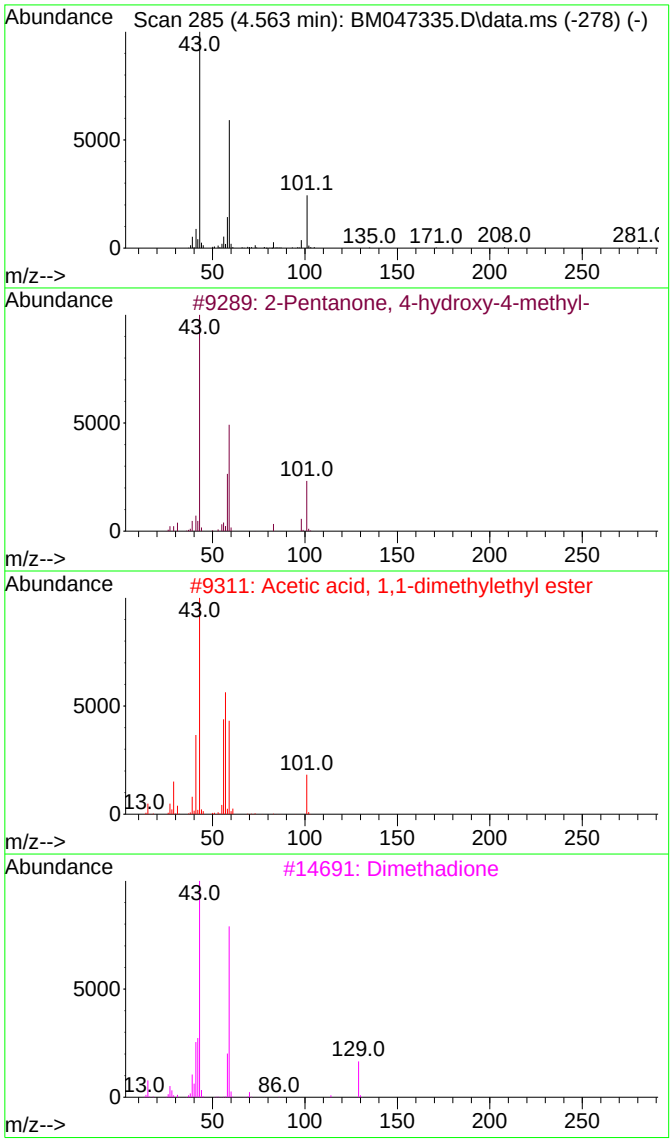
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

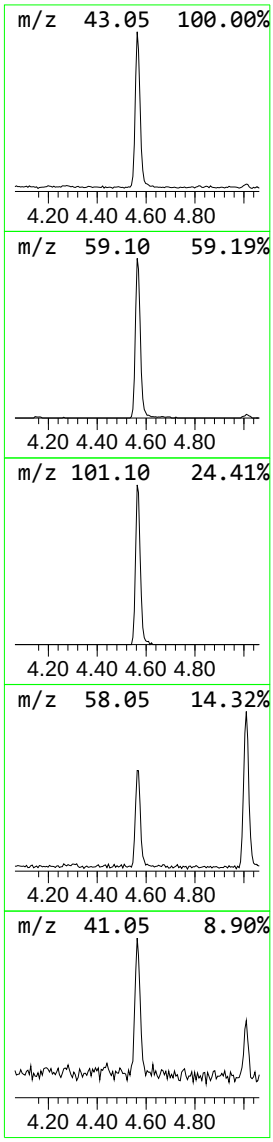
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	2.53 ng	204809	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	Dimethadione	129	C5H7NO3	000695-53-4	40
4	Tetraglyme	222	C10H22O5	000143-24-8	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





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Acq On : 23 Aug 2024 16:08
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Instrument :
BNA_M
ClientSampleId :
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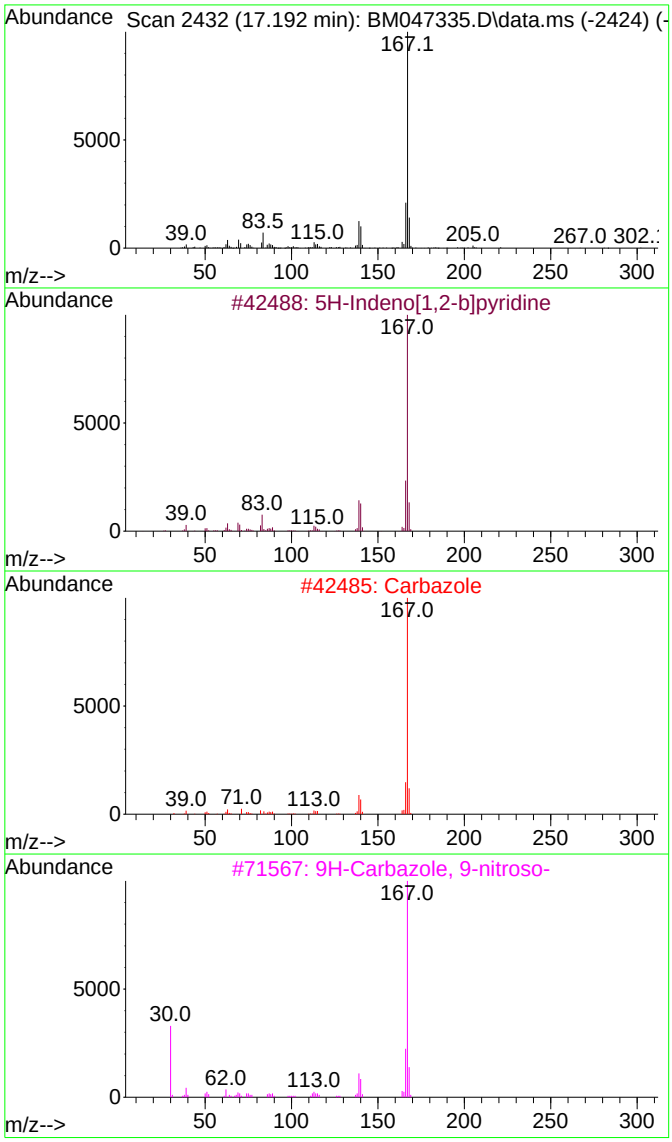
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

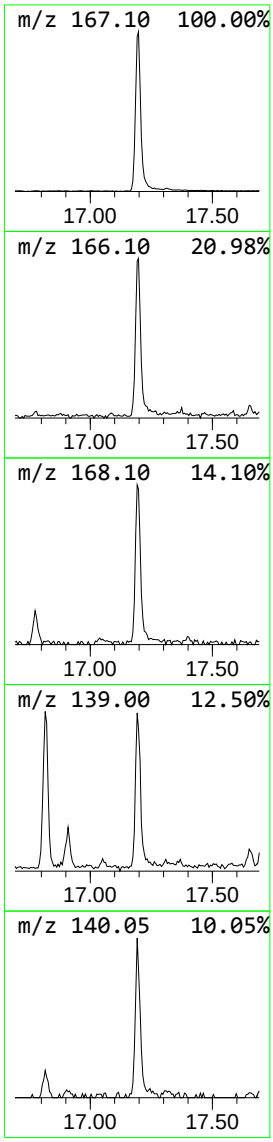
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 5H-Indeno[1,2-b]pyridine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.192	2.08 ng	337198	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	95
2	Carbazole	167	C12H9N	000086-74-8	93
3	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	80
4	2-Azafluorene	167	C12H9N	000244-40-6	64
5	ethanone, 1-(9H-carbazol-9-yl)-	209	C14H11NO	1000400-59-5	64





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Sample : P3686-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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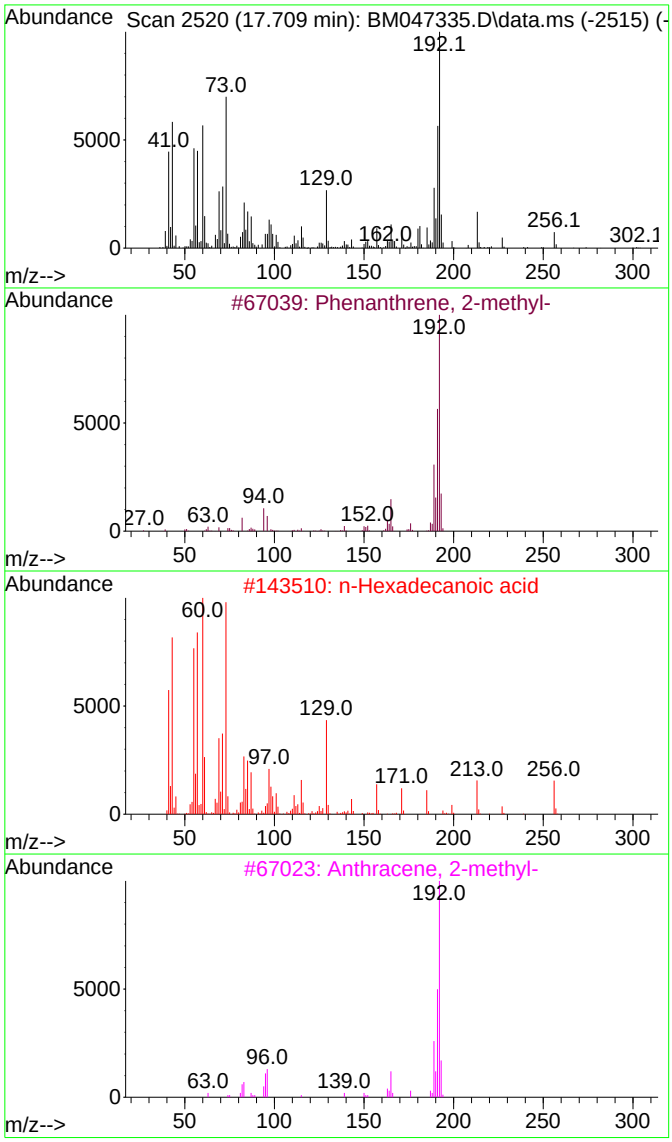
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

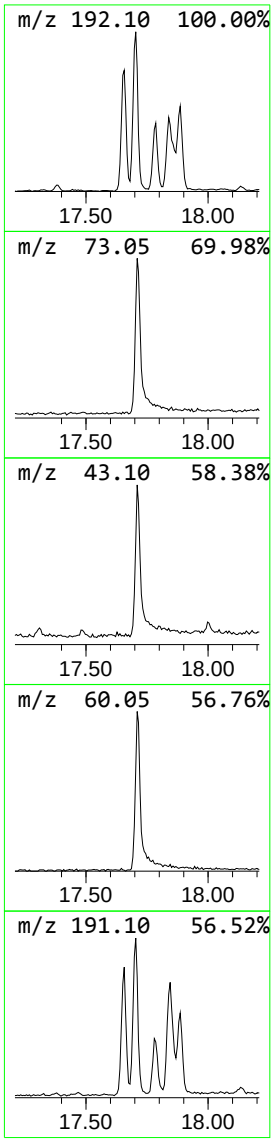
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	5.02 ng	812351	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





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Data File : BM047335.D
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Sample : P3686-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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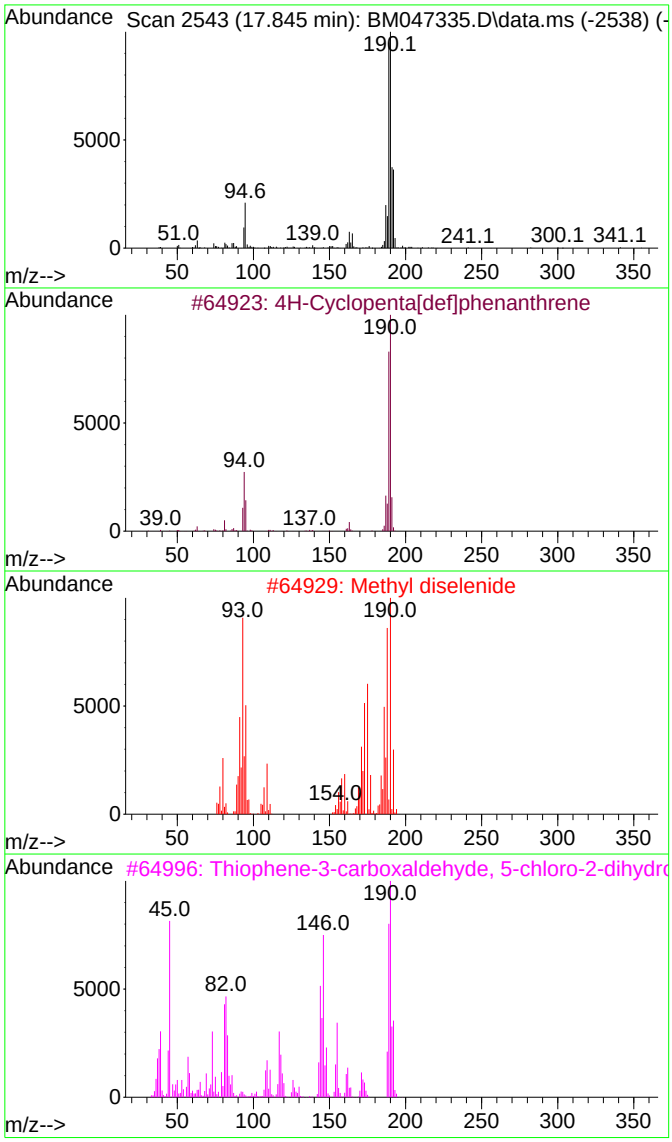
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

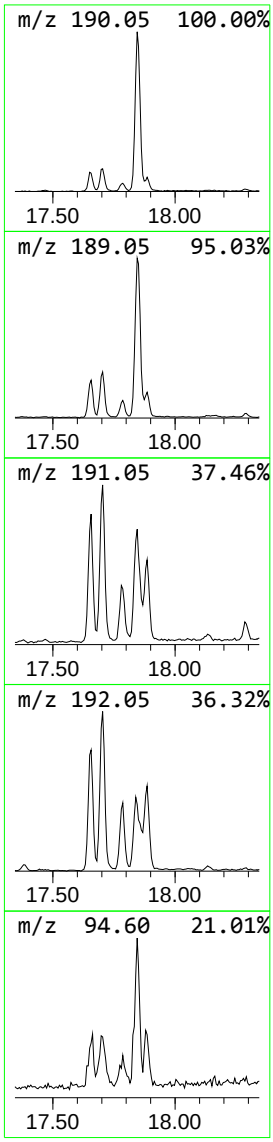
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.845	3.06 ng	495270	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Methyl diselenide	190	C2H6Se2	007101-31-7	55
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45





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-...	4.563	2.5	ng	204809	1	7.351	1620580	20.0
5H-Indeno[1,2-b...	17.192	2.1	ng	337198	4	16.774	3239330	20.0
Phenanthrene, 2...	17.709	5.0	ng	812351	4	16.774	3239330	20.0
4H-Cyclopenta[d...	17.845	3.1	ng	495270	4	16.774	3239330	20.0