LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
Data File : BM039409.D
Acq On : 12 Apr 2023 18:39
Operator : CG/JU
Sample : 02284-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-2-041123

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: BM039409.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	308	rVB	156438	218626	4.73%	0.498%
2	5.446	377	384	399	rBV	1353073	2166863	46.90%	4.936%
3	7.069	653	660	674	rBV	1298118	2195208	47.51%	5.000%
4	7.857	784	794	809	rBV	886667	1505268	32.58%	3.429%
5	8.404	881	887	896	rBV	28953	56148	1.22%	0.128%
6	9.034	987	994	1010	rBV	742299	1399211	30.29%	3.187%
7	10.669	1259	1272	1287	rBV	1193461	2169612	46.96%	4.942%
8	11.363	1379	1390	1398	rBV	12510	48576	1.05%	0.111%
9	12.087	1506	1513	1519	rBV3	22675	48895	1.06%	0.111%
10	12.551	1587	1592	1603	rVB4	25662	73491	1.59%	0.167%
11	13.139	1684	1692	1701	rBV	2056829	3250743	70.36%	7.405%
12	13.328	1721	1724	1732	rVB3	27426	53588	1.16%	0.122%
13	13.833	1805	1810	1815	rBV2	41002	78026	1.69%	0.178%
14	13.980	1829	1835	1840	rBV2	53437	110800	2.40%	0.252%
15	14.239	1873	1879	1891	rBV	324436	565580	12.24%	1.288%
16	14.404	1903	1907	1914	rVB	38460	53145	1.15%	0.121%
17	14.516	1915	1926	1933	rBV	1738441	2664022	57.66%	6.068%
18	14.580	1933	1937	1944	rVB	86747	145084	3.14%	0.330%
19	14.728	1957	1962	1971	rVB8	22640	56495	1.22%	0.129%
20	14.916	1990	1994	1999	rVB	45291	60088	1.30%	0.137%
21	15.127	2025	2030	2034	rBV4	38456	70283	1.52%	0.160%
22	15.298	2054	2059	2063	rBV6	30839	62874	1.36%	0.143%
23	15.386	2071	2074	2081	rVB	48766	77929	1.69%	0.178%
24	15.569	2100	2105	2116	rVB	120288	249455	5.40%	0.568%
25	15.769	2135	2139	2149	rVB5	48716	96144	2.08%	0.219%
26	15.880	2151	2158	2170	rVB	423250	709851	15.36%	1.617%
27	16.010	2171	2180	2189	rBV	1549690	2380555	51.53%	5.422%
28	16.239	2213	2219	2228	rVB2	113270	231739	5.02%	0.528%
29	16.439	2250	2253	2260	rVB	43380	58729	1.27%	0.134%
30	16.798	2311	2314	2318	rBV3	49461	67211	1.45%	0.153%
31	17.080	2357	2362	2370	rVB2	84483	209592	4.54%	0.477%
32	17.269	2388	2394	2397	rBV	1902276	2813212	60.89%	6.408%
33	17.310	2397	2401	2411	rVB	988540	1461537	31.63%	3.329%
34	17.398	2411	2416	2422	rBV	490417	722453	15.64%	1.646%
35	17.680	2461	2464	2469	rVB	64550	92926	2.01%	0.212%
36	18.168	2539	2547	2549	rBV2	547626	984773	21.32%	2.243%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
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Operator : CG/JU
Sample : 02284-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-2-041123

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	18.274	2562	2565	2570	rVB	139835	168443	3.65%	0.384%
38	18.339	2571	2576	2580	rBV2	345763	626849	13.57%	1.428%
39	19.063	2695	2699	2705	rBV3	215931	428995	9.29%	0.977%
40	19.327	2739	2744	2750	rBV	2201160	2974049	64.37%	6.774%
41	19.445	2762	2764	2767	rBV	196254	233395	5.05%	0.532%
42	19.692	2797	2806	2814	rBV	2273747	3708385	80.27%	8.447%
43	19.892	2836	2840	2846	rBV	3127833	3933098	85.13%	8.959%
44	21.456	3100	3106	3110	rBV2	2578144	4620075	100.00%	10.524%

Sum of corrected areas: 43902021

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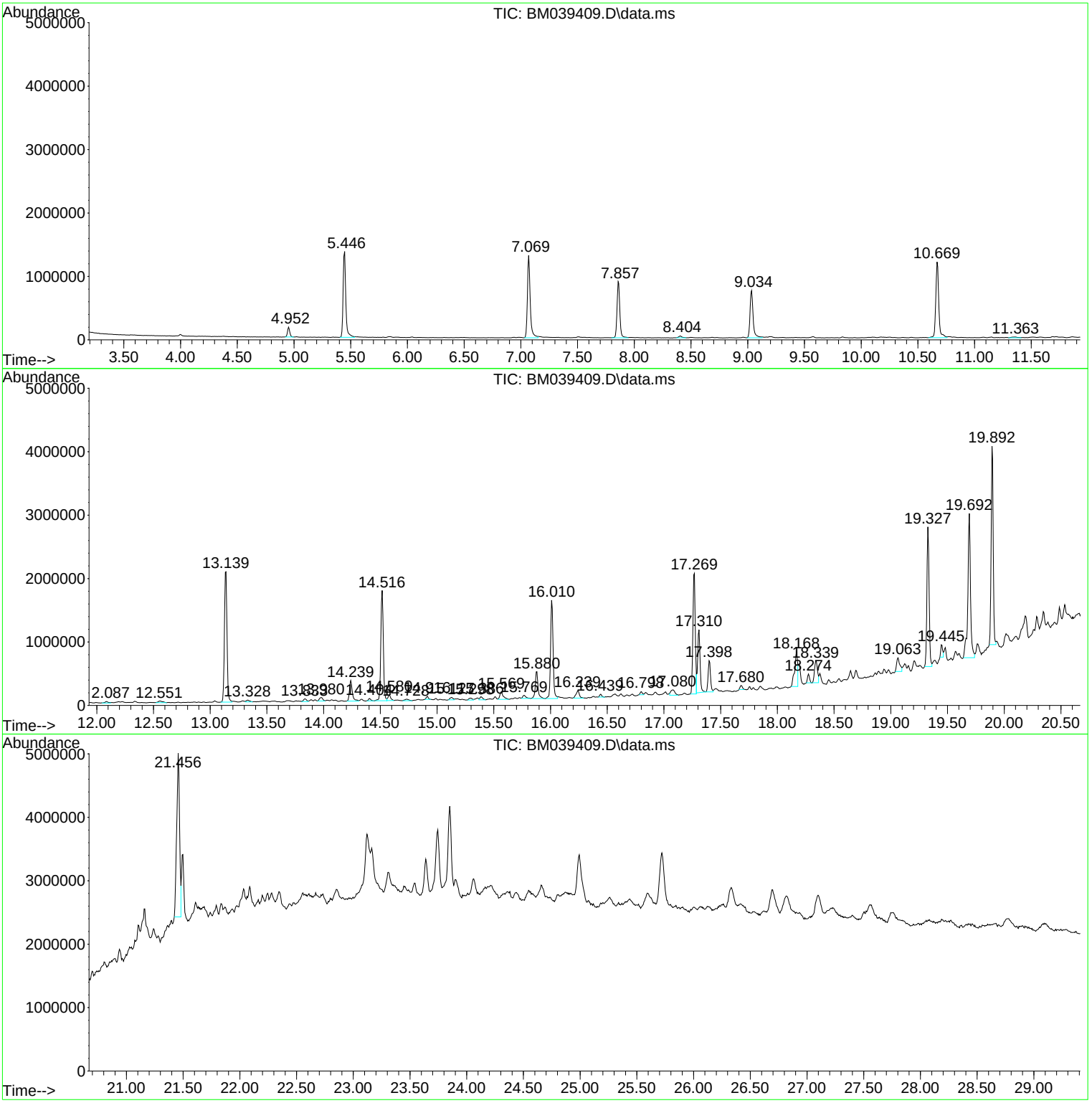
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-2-041123

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\BM041223\
Data File : BM039409.D
Acq On : 12 Apr 2023 18:39
Operator : CG/JU
Sample : 02284-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-2-041123

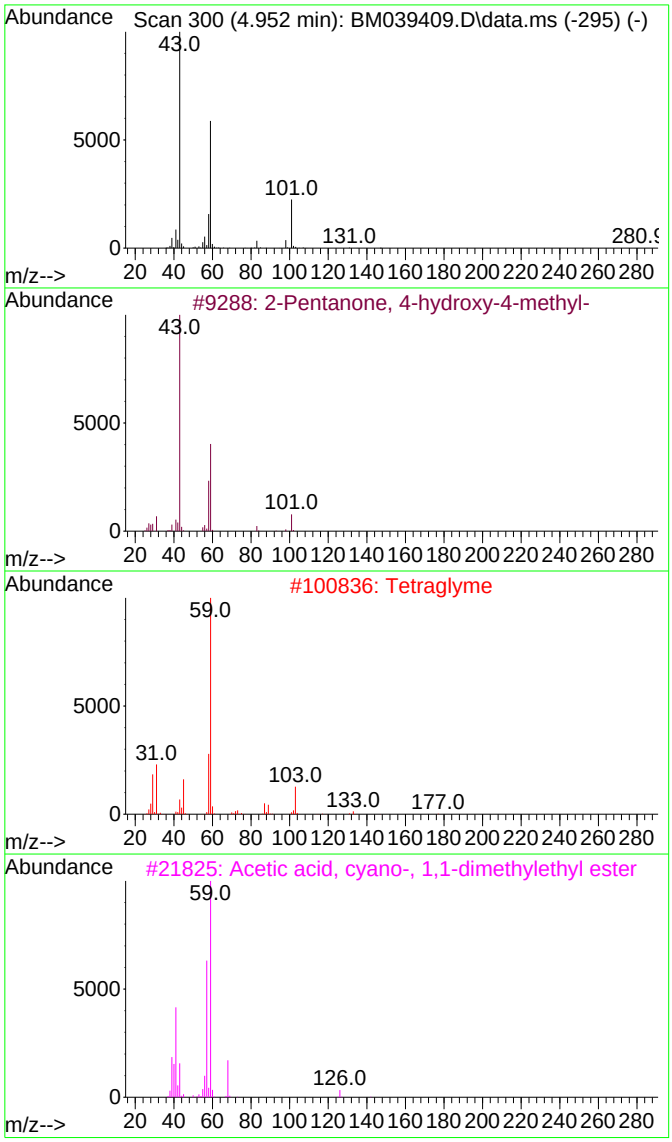
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

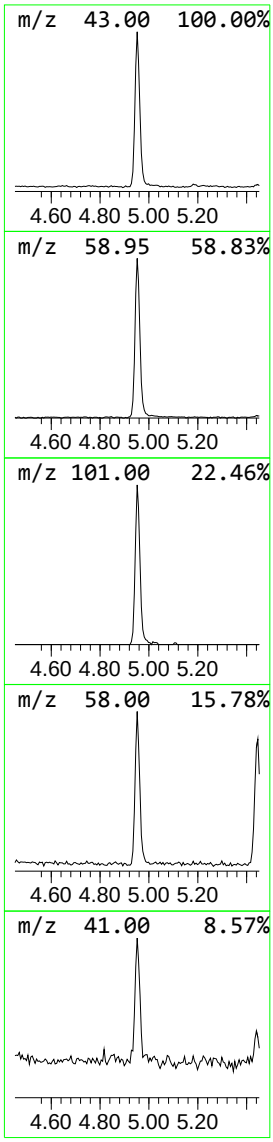
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.952	2.90 ng	218626	1,4-Dichlorobenzene-d4	7.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Tetraglyme	222	C10H22O5	000143-24-8	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Sample : 02284-01 2X
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

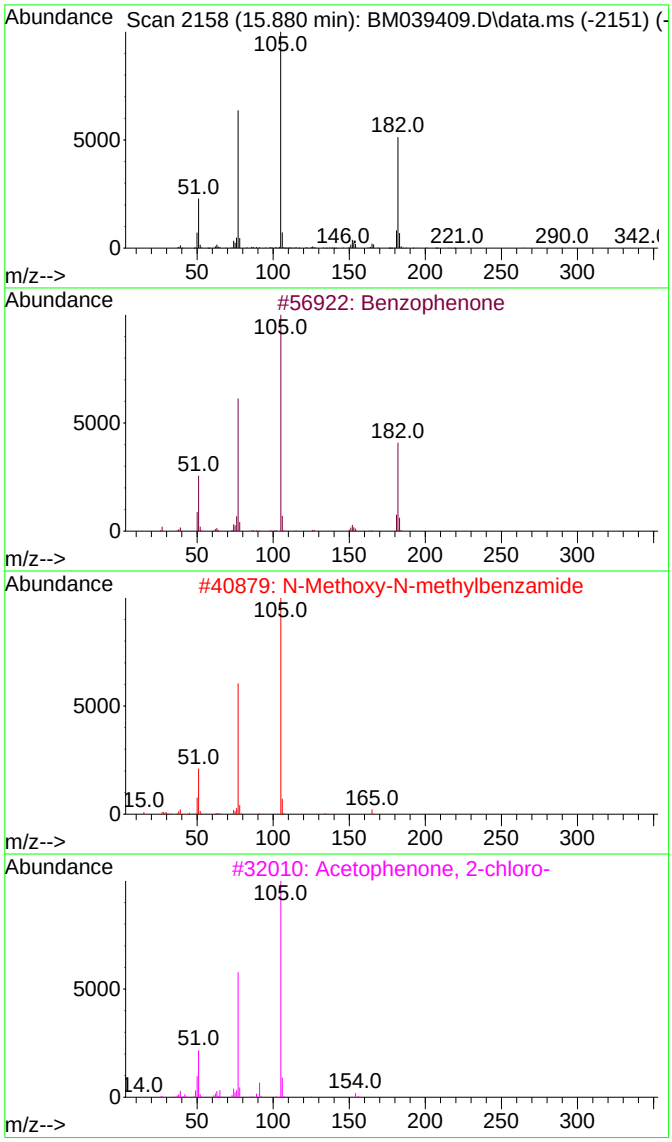
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

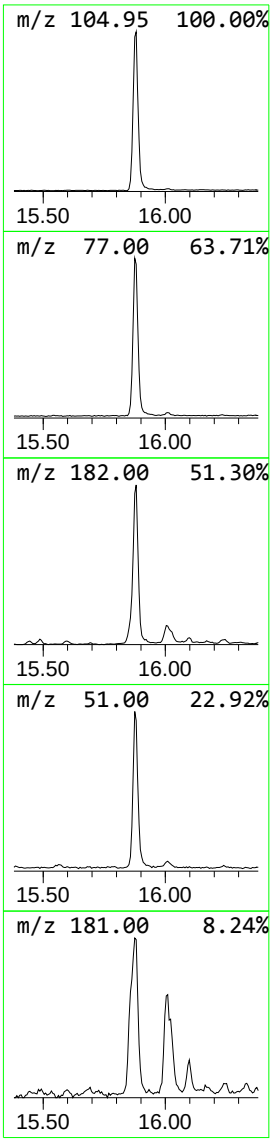
****

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	5.33 ng	709851	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	60
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47





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Sample : 02284-01 2X
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

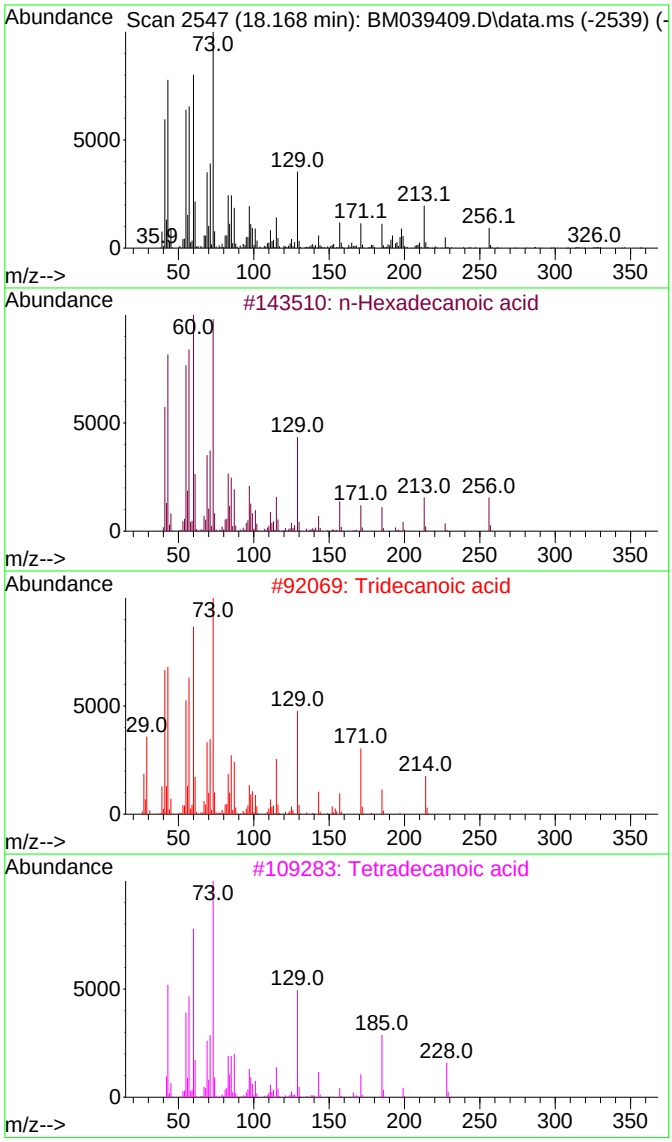
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

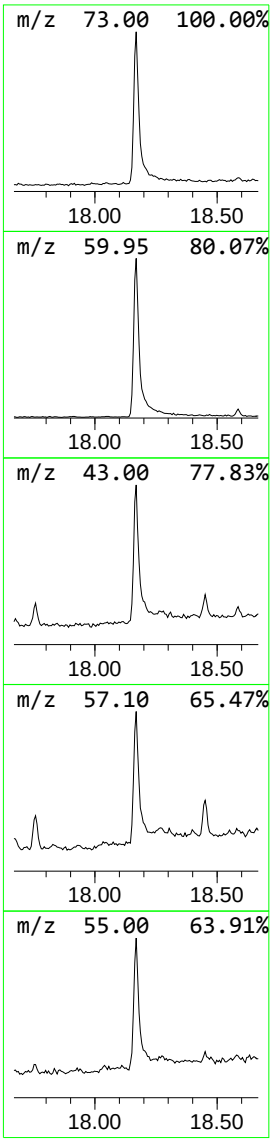
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	7.00 ng	984773	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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Operator : CG/JU
Sample : 02284-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-2-041123

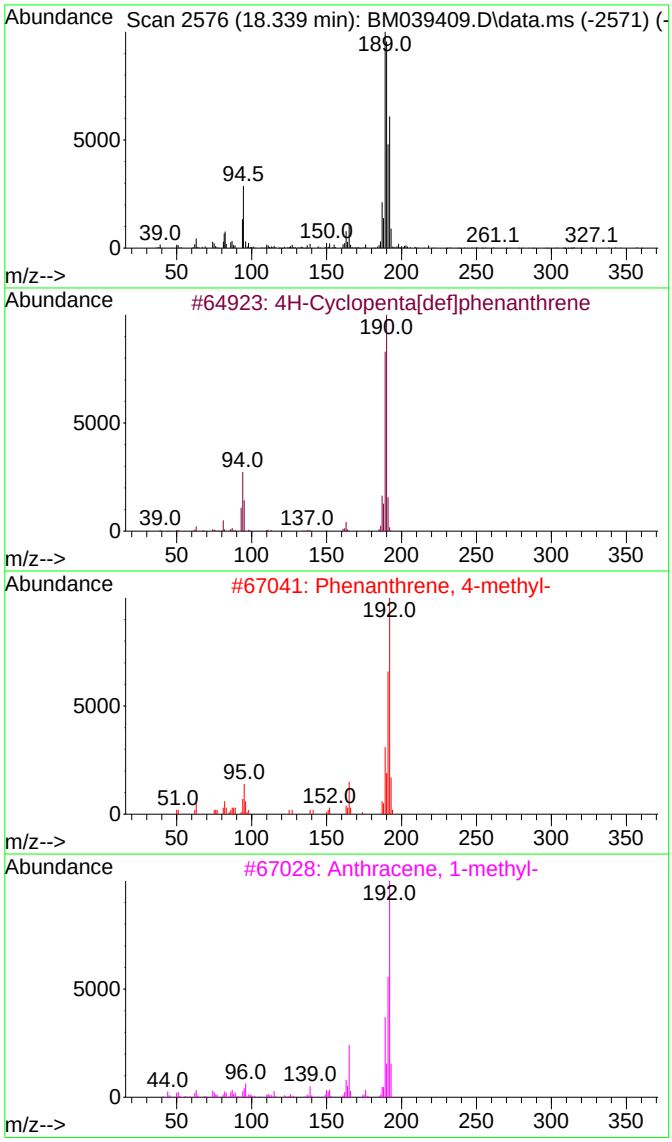
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

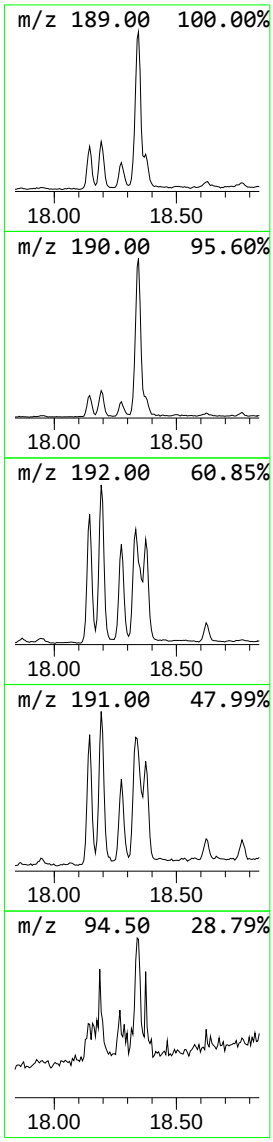
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.339	4.46 ng	626849	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	25
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	20
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	20





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-2-041123

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

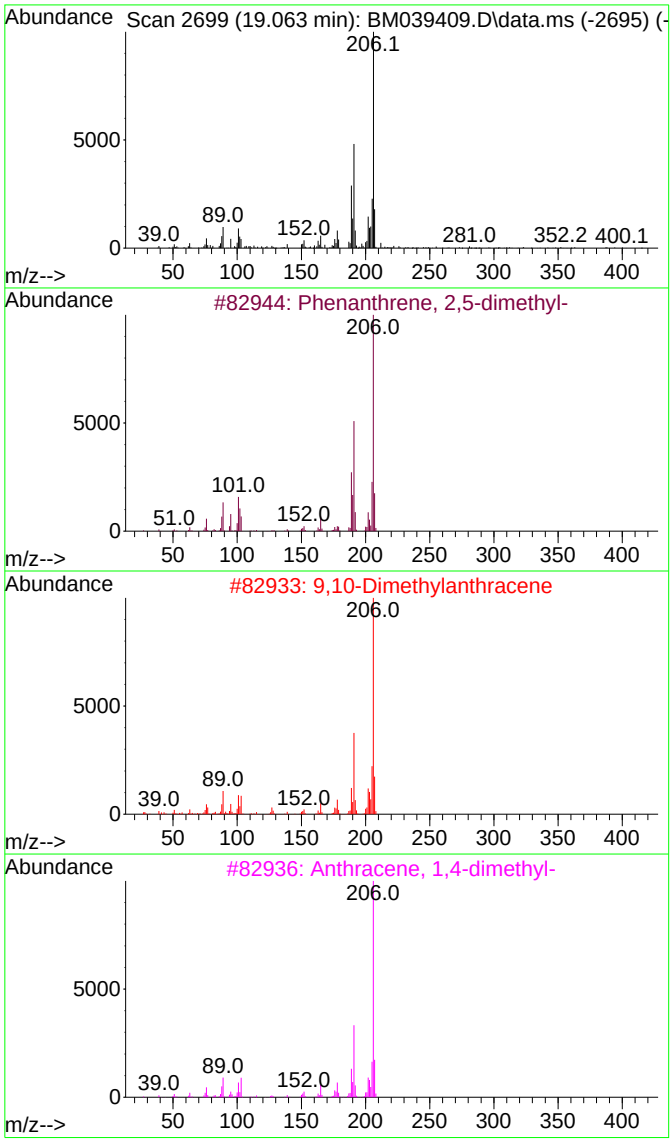
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

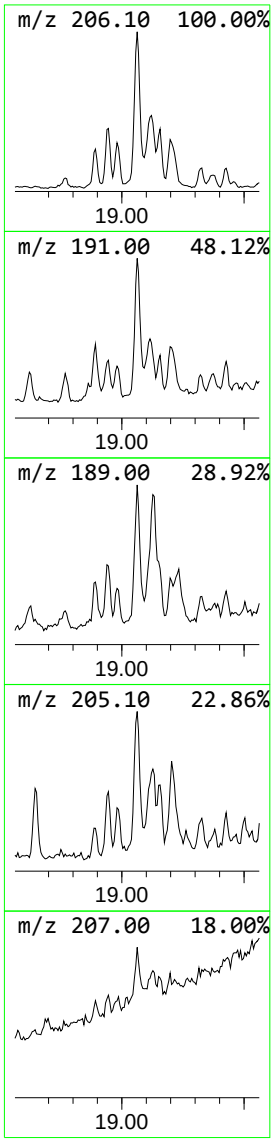
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.063	3.05 ng	428995	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	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041223\
Data File : BM039409.D
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Operator : CG/JU
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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	2.9	ng	218626	1	7.857	1505270	20.0
Benzophenone	15.880	5.3	ng	709851	3	14.516	2664020	20.0
n-Hexadecanoic ...	18.169	7.0	ng	984773	4	17.269	2813210	20.0
4H-Cyclopenta[d...	18.339	4.5	ng	626849	4	17.269	2813210	20.0
Phenanthrene, 2...	19.063	3.0	ng	428995	4	17.269	2813210	20.0