LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047287.D
Acq On : 21 Aug 2024 02:12
Operator : RC/JU
Sample : P3643-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

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: BM047287.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	76	rBV	91222	138471	2.17%	0.210%
2	4.569	279	286	297	rVB	230555	325694	5.11%	0.493%
3	5.016	355	362	374	rBV	3535067	5059513	79.34%	7.655%
4	6.575	619	627	641	rBV	3291024	5163127	80.96%	7.812%
5	6.993	693	698	709	rBV	44664	97347	1.53%	0.147%
6	7.357	754	760	767	rBV	1095927	1653188	25.92%	2.501%
7	8.504	945	955	967	rBV	2056952	3281184	51.45%	4.965%
8	9.087	1048	1054	1064	rBV	94033	163692	2.57%	0.248%
9	10.110	1219	1228	1235	rBV	1345269	2154190	33.78%	3.259%
10	10.687	1322	1326	1335	rVB4	39040	73377	1.15%	0.111%
11	10.875	1351	1358	1369	rBV	188734	387573	6.08%	0.586%
12	12.622	1648	1655	1672	rBV	3890350	5781468	90.66%	8.748%
13	14.016	1886	1892	1898	rBV	1874923	2707838	42.46%	4.097%
14	14.080	1898	1903	1913	rVB	188872	299480	4.70%	0.453%
15	14.251	1926	1932	1933	rBV	896003	1028929	16.13%	1.557%
16	14.269	1933	1935	1944	rVB	1070336	1419059	22.25%	2.147%
17	14.427	1957	1962	1968	rVB	59586	88324	1.39%	0.134%
18	15.080	2067	2073	2078	rBV	142231	205141	3.22%	0.310%
19	15.527	2142	2149	2160	rBV	3329756	4991149	78.27%	7.552%
20	16.086	2235	2244	2249	rBV5	31010	85636	1.34%	0.130%
21	16.598	2324	2331	2341	rVB	88854	171185	2.68%	0.259%
22	16.780	2356	2362	2366	rBV	2130764	3005492	47.13%	4.548%
23	16.821	2366	2369	2377	rVV	1331456	1854160	29.08%	2.805%
24	16.916	2377	2385	2392	rVV	383730	604787	9.48%	0.915%
25	16.980	2392	2396	2402	rVV	45470	76917	1.21%	0.116%
26	17.198	2422	2433	2448	rBV2	146446	312998	4.91%	0.474%
27	17.657	2505	2511	2516	rBV	111903	180865	2.84%	0.274%
28	17.716	2516	2521	2529	rVV2	535720	855870	13.42%	1.295%
29	17.786	2529	2533	2538	rVV	96237	180291	2.83%	0.273%
30	17.851	2539	2544	2548	rVV3	242723	413132	6.48%	0.625%
31	17.892	2548	2551	2560	rVB	92876	146562	2.30%	0.222%
32	18.174	2594	2599	2602	rBV	81551	110533	1.73%	0.167%
33	18.215	2603	2606	2610	rVB	61071	76301	1.20%	0.115%
34	18.421	2634	2641	2646	rBV7	32513	72142	1.13%	0.109%
35	18.592	2665	2670	2674	rBV2	66637	112756	1.77%	0.171%
36	18.680	2677	2685	2690	rVV4	96392	221837	3.48%	0.336%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047287.D
Acq On : 21 Aug 2024 02:12
Operator : RC/JU
Sample : P3643-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

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	18.733	2690	2694	2704	rVB5	43587	97174	1.52%	0.147%
38	18.857	2710	2715	2720	rBV	1844204	2402485	37.67%	3.635%
39	19.015	2738	2742	2747	rBV2	172081	251974	3.95%	0.381%
40	19.104	2754	2757	2761	rVB	55079	73650	1.15%	0.111%
41	19.221	2769	2777	2785	rBV	1393189	2319840	36.38%	3.510%
42	19.292	2786	2789	2797	rVB3	84886	172370	2.70%	0.261%
43	19.445	2810	2815	2827	rVB	5174478	6377136	100.00%	9.649%
44	19.562	2830	2835	2841	rVB3	59045	150679	2.36%	0.228%
45	19.692	2853	2857	2860	rBV4	71309	127673	2.00%	0.193%
46	19.733	2860	2864	2870	rVB	229296	309315	4.85%	0.468%
47	19.833	2877	2881	2885	rBV2	179171	229033	3.59%	0.347%
48	19.886	2886	2890	2894	rVV2	107313	163760	2.57%	0.248%
49	20.074	2919	2922	2927	rBV3	57859	94887	1.49%	0.144%
50	20.492	2990	2993	2998	rVB2	73853	97088	1.52%	0.147%
51	20.651	3017	3020	3023	rBV	104751	117774	1.85%	0.178%
52	20.692	3024	3027	3029	rBV2	86288	87277	1.37%	0.132%
53	20.721	3030	3032	3034	rBV2	65661	76934	1.21%	0.116%
54	20.756	3034	3038	3042	rVV3	238552	343021	5.38%	0.519%
55	21.015	3075	3082	3086	rBV2	2217430	3722615	58.37%	5.633%
56	21.056	3086	3089	3099	rVB	643692	871848	13.67%	1.319%
57	21.186	3108	3111	3115	rVB	143709	168955	2.65%	0.256%
58	22.868	3392	3397	3403	rBV	378384	924560	14.50%	1.399%
59	23.586	3514	3519	3527	rVB	347045	722249	11.33%	1.093%
60	23.709	3533	3540	3548	rBV	1148817	2687676	42.15%	4.067%

Sum of corrected areas: 66090181

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
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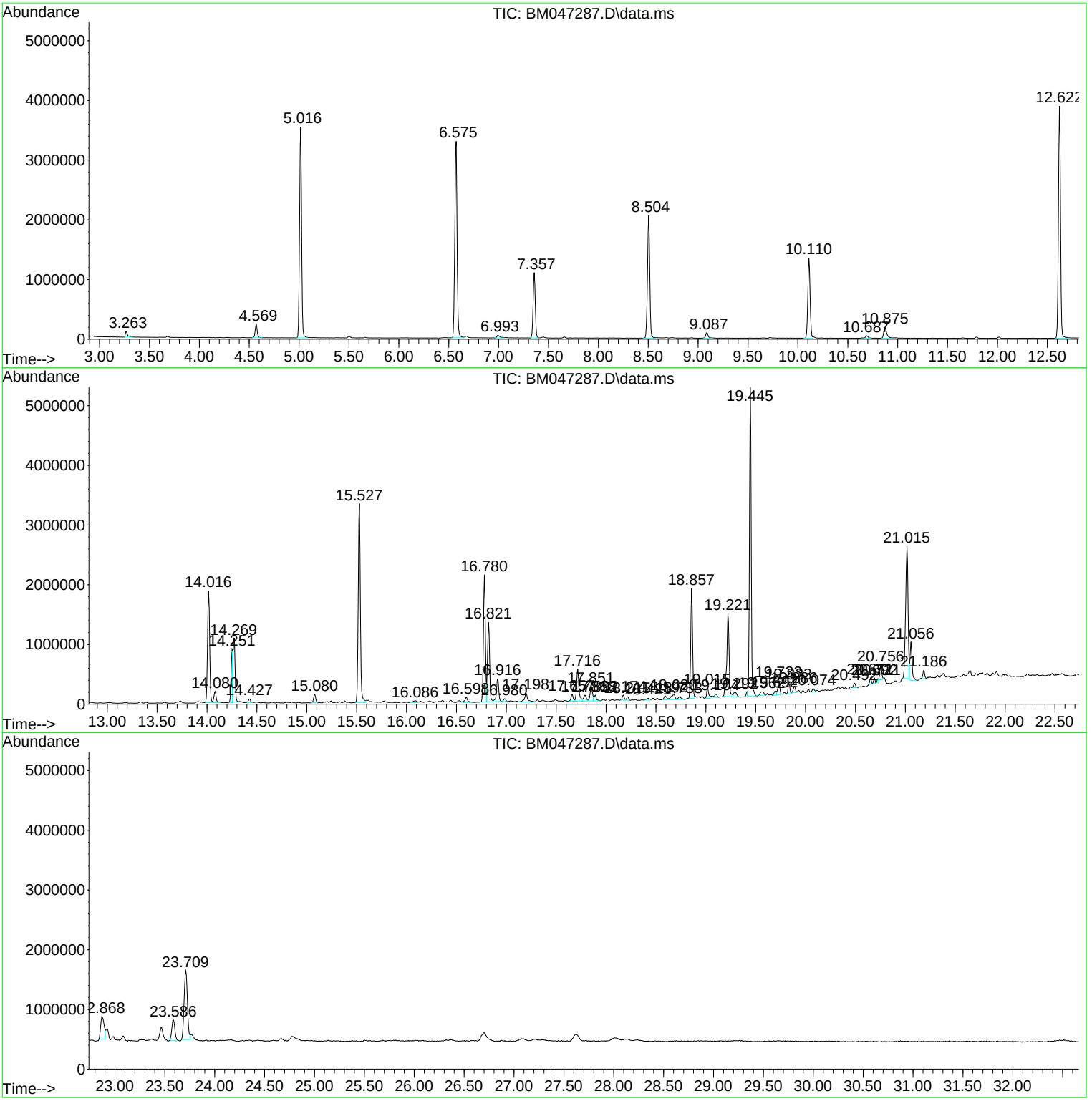
Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

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 : BM047287.D
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Operator : RC/JU
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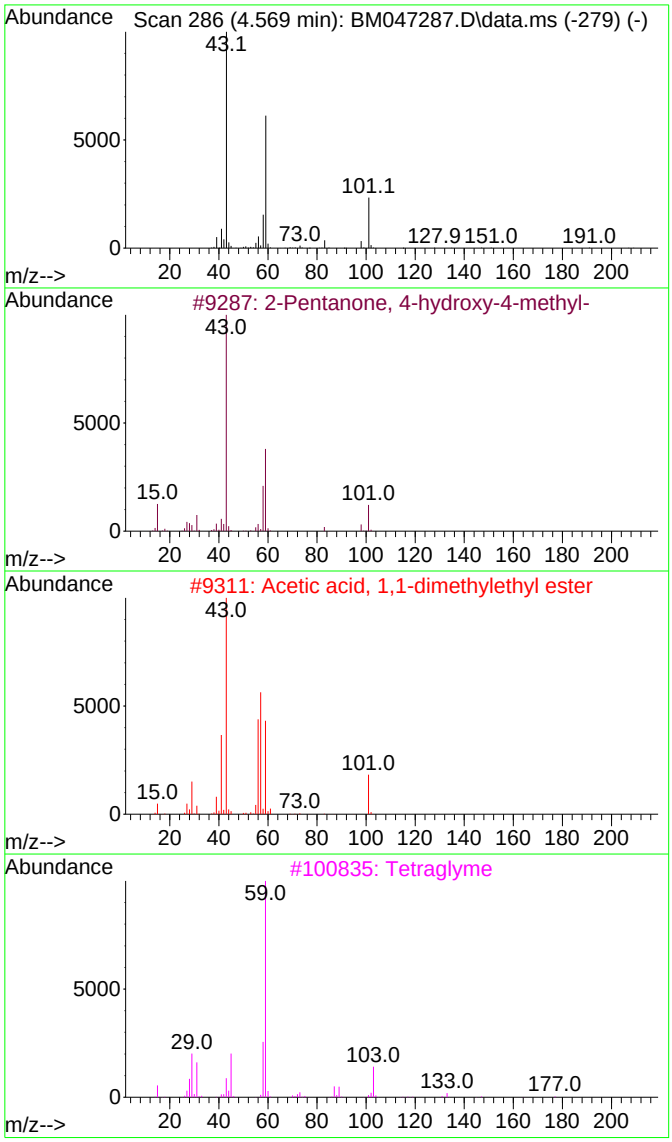
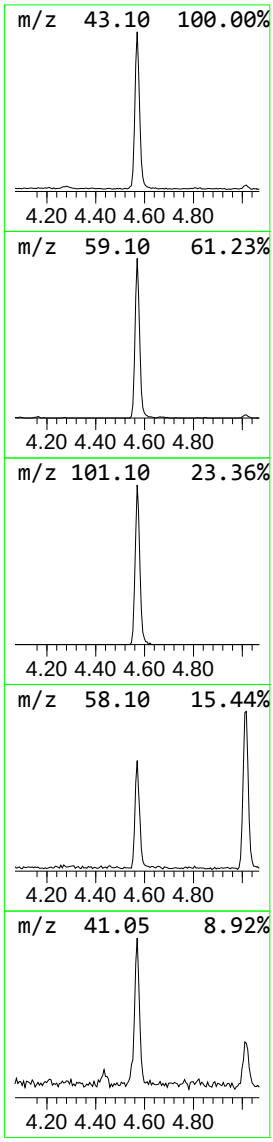
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.94 ng	325694	1,4-Dichlorobenzene-d4	7.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Tetraglyme	222	C10H22O5	000143-24-8	37
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047287.D
Acq On : 21 Aug 2024 02:12
Operator : RC/JU
Sample : P3643-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

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

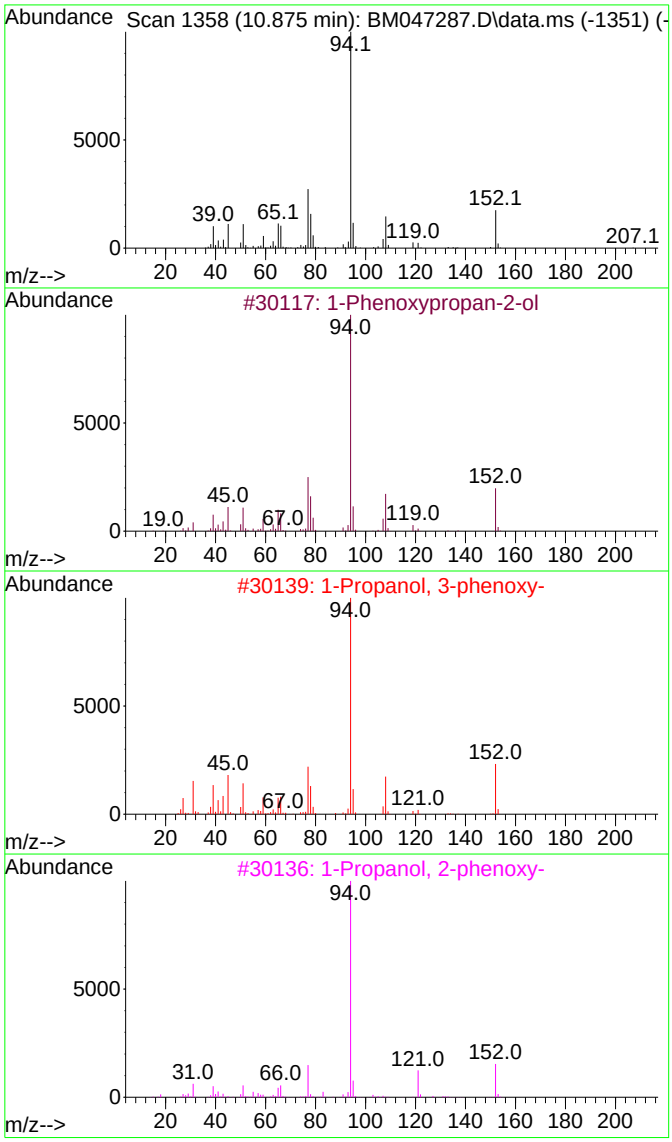
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

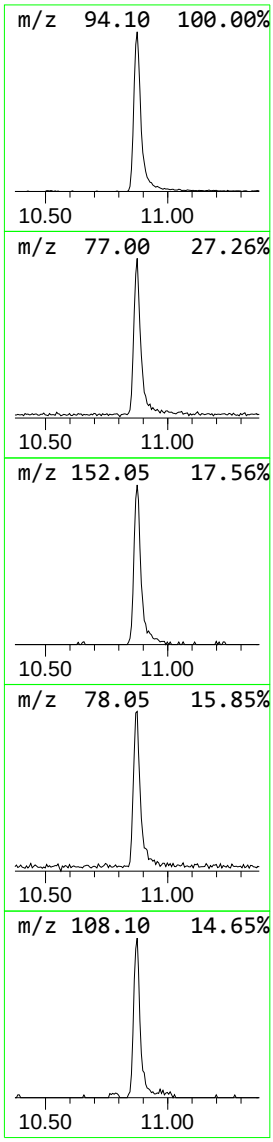
****

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	3.60 ng	387573	Naphthalene-d8	10.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
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Sample : P3643-11
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

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

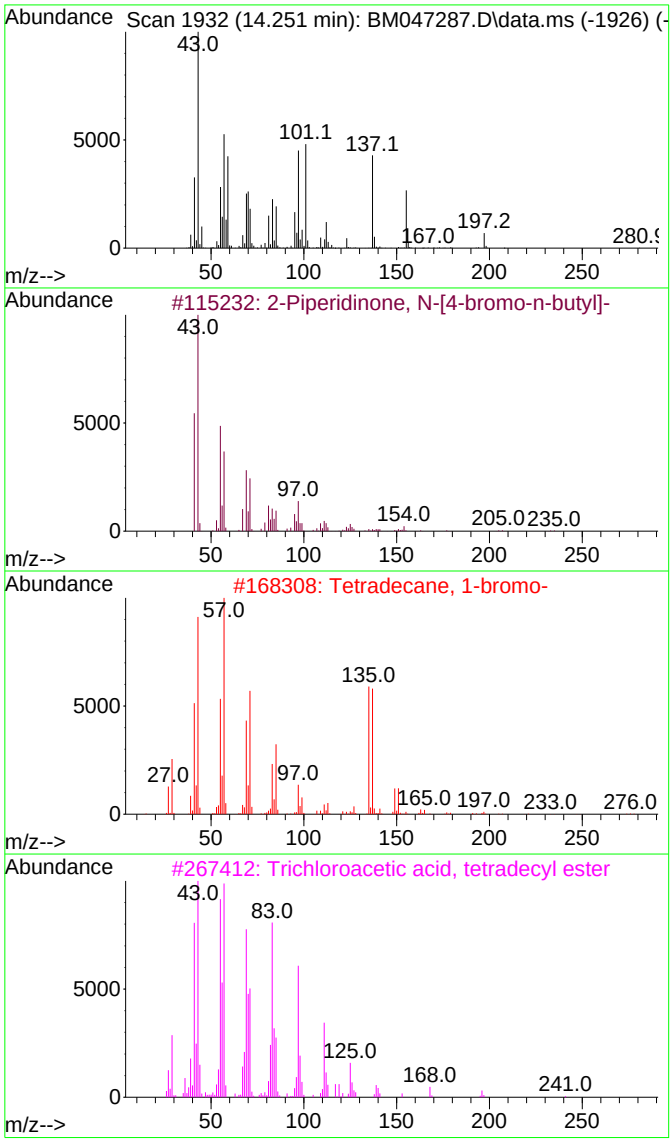
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

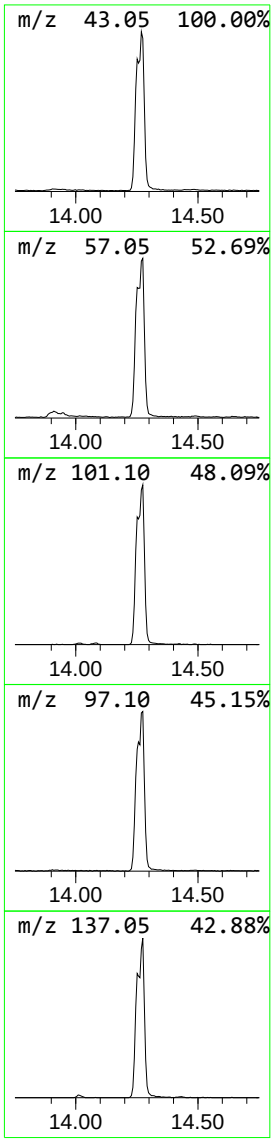
****

Peak Number 4 unknown14.251 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	7.60 ng	1028930	Acenaphthene-d10	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	16
2	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	14
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	12
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5	2-Butanol, 2-methyl-, acetate	130	C7H14O2	000625-16-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047287.D
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Operator : RC/JU
Sample : P3643-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

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
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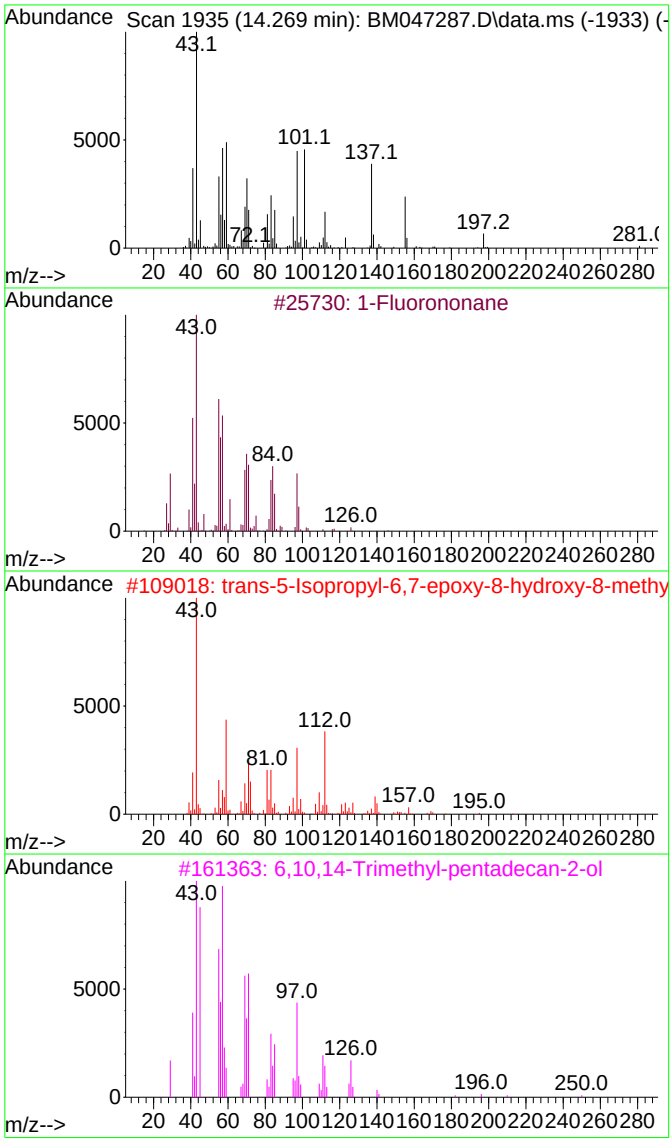
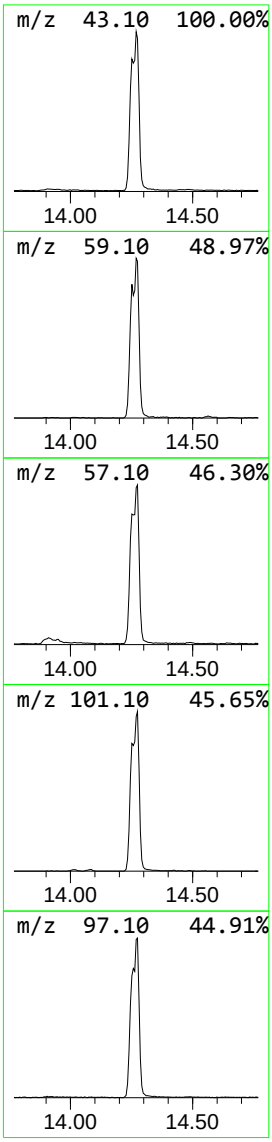
****

Peak Number 5 unknown14.269 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	10.48 ng	1419060	Acenaphthene-d10	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Fluorononane	146	C9H19F	000463-18-3	14
2	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
3	6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	10
4	2-Hydroxypyridine-3-carboximidamide	137	C6H7N3O	1000411-26-0	9
5	Decane, 1-bromo-	220	C10H21Br	000112-29-8	9





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Data File : BM047287.D
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Sample : P3643-11
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ClientSampleId :
921-J-SD-0-0.5-081524

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

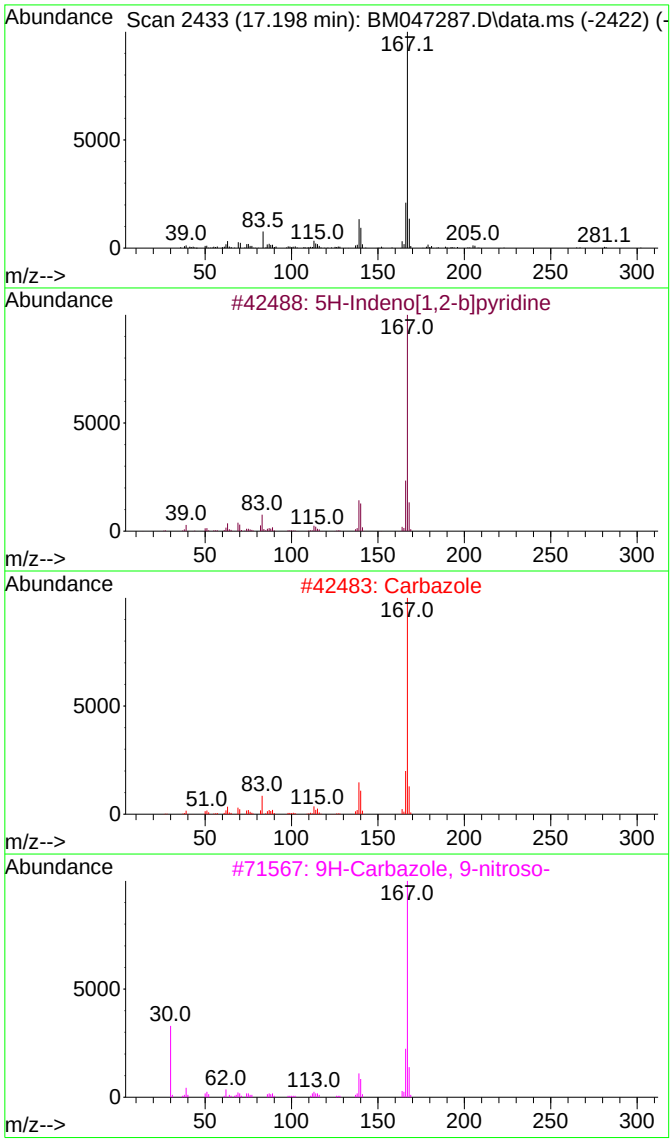
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

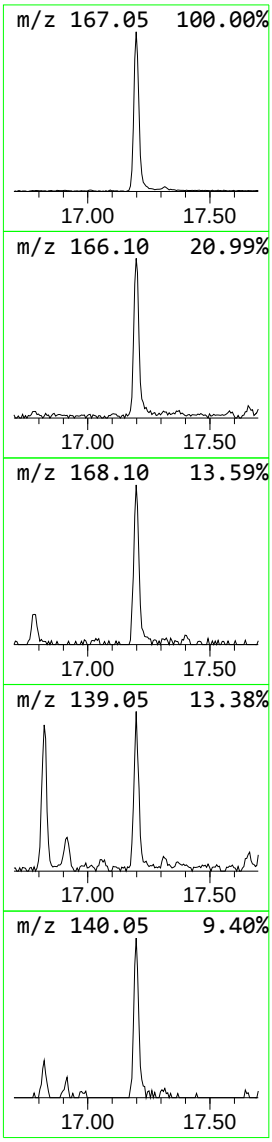
****

Peak Number 6 5H-Indeno[1,2-b]pyridine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	2.08 ng	312998	Phenanthrene-d10	16.780

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	95
3	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	86
4	2-Azafluorene	167	C12H9N	000244-40-6	72
5	1-Naphthaleneacetonitrile	167	C12H9N	000132-75-2	68





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BNA_M
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921-J-SD-0-0.5-081524

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

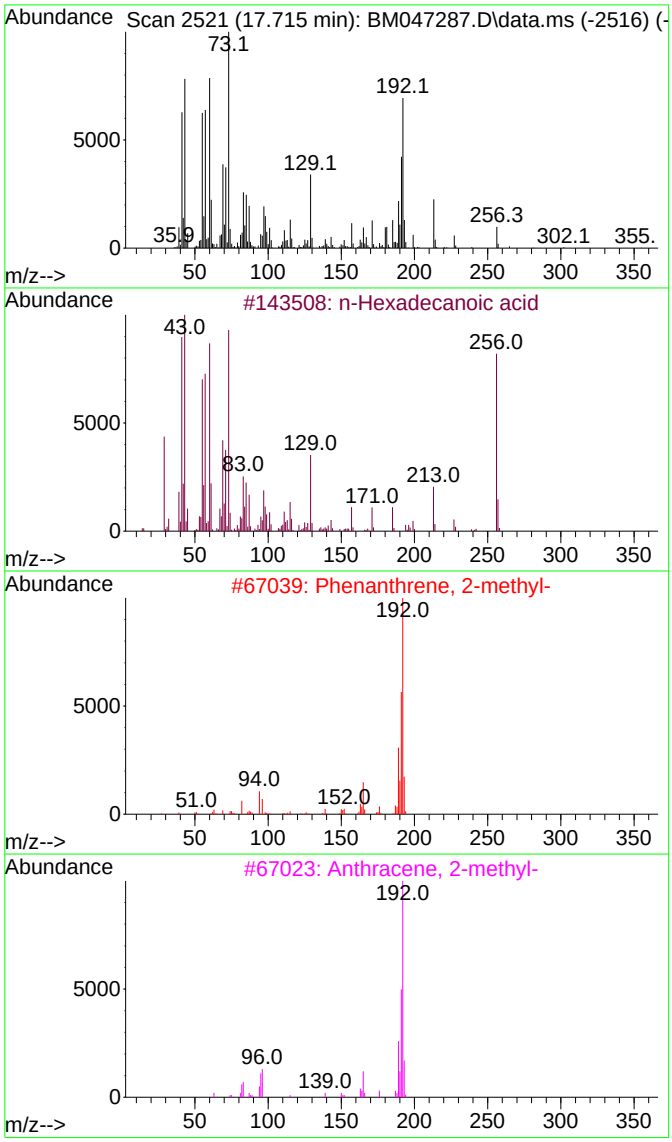
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

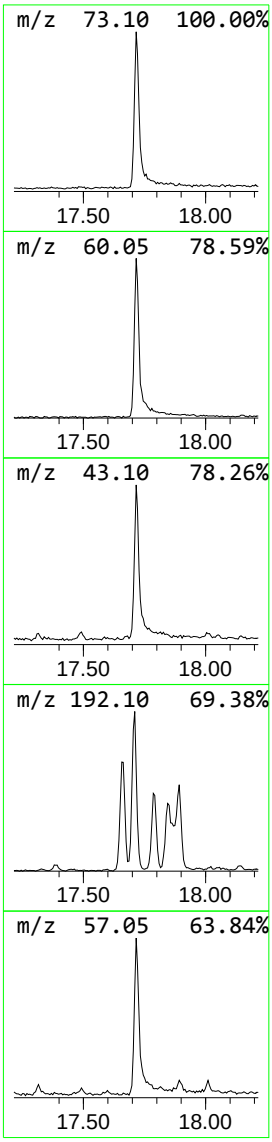
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	5.70 ng	855870	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047287.D
Acq On : 21 Aug 2024 02:12
Operator : RC/JU
Sample : P3643-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

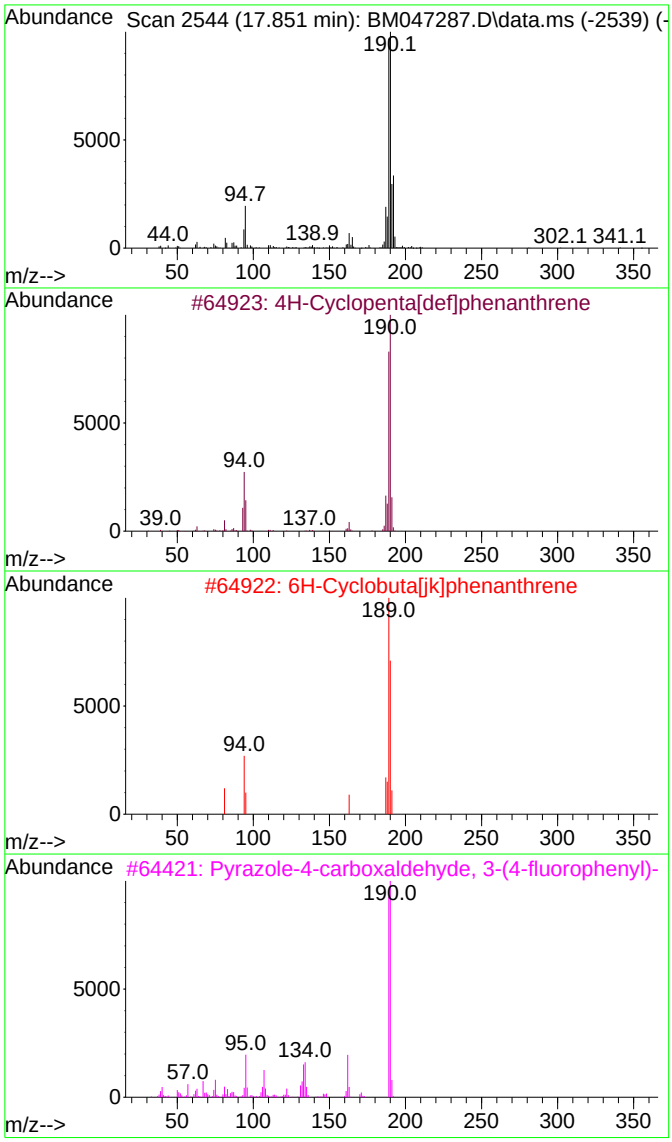
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

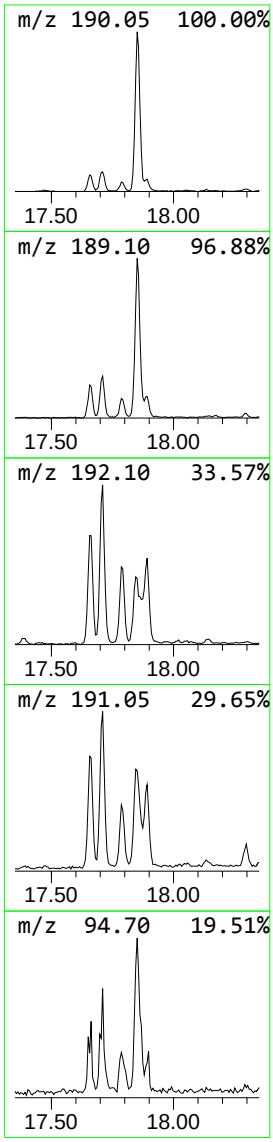
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.851	2.75 ng	413132	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
4	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047287.D
Acq On : 21 Aug 2024 02:12
Operator : RC/JU
Sample : P3643-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
921-J-SD-0-0.5-081524

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.569	3.9	ng	325694	1	7.357	1653190	20.0
1-Phenoxypropan...	10.875	3.6	ng	387573	2	10.110	2154190	20.0
unknown14.251	14.251	7.6	ng	1028930	3	14.016	2707840	20.0
unknown14.269	14.269	10.5	ng	1419060	3	14.016	2707840	20.0
5H-Indeno[1,2-b...	17.198	2.1	ng	312998	4	16.780	3005490	20.0
n-Hexadecanoic ...	17.715	5.7	ng	855870	4	16.780	3005490	20.0
4H-Cyclopenta[d...	17.851	2.8	ng	413132	4	16.780	3005490	20.0