

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091624\
 Data File : BM047535.D
 Acq On : 16 Sep 2024 12:56
 Operator : RC/JU
 Sample : P3845-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PT-BN-WP

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-BM091424.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047535.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.628	87	92	110	rVB	3229687	4268272	9.59%	0.689%
2	4.957	313	318	328	rVB	439110	643242	1.45%	0.104%
3	5.422	390	397	407	rBV	8395171	11653595	26.20%	1.881%
4	7.010	659	667	687	rBV	8324499	12777822	28.72%	2.062%
5	7.269	703	711	722	rBV	5569121	7939072	17.85%	1.281%
6	7.739	783	791	799	rBV	9870174	15287473	34.36%	2.467%
7	7.845	802	809	819	rBV	1328831	2145192	4.82%	0.346%
8	8.375	891	899	908	rBV	2569281	5944582	13.36%	0.959%
9	8.657	939	947	961	rVB	6106532	9317787	20.94%	1.504%
10	8.934	986	994	1000	rBV	6730985	10607876	23.84%	1.712%
11	9.004	1000	1006	1011	rVV	4887477	7710330	17.33%	1.244%
12	10.645	1277	1285	1288	rBV	1863643	3068967	6.90%	0.495%
13	10.698	1288	1294	1303	rVB	14667334	24022245	54.00%	3.877%
14	10.992	1336	1344	1352	rBV	4834785	7479441	16.81%	1.207%
15	12.310	1558	1568	1576	rBV	10256294	15623007	35.12%	2.521%
16	12.527	1597	1605	1613	rVB	20215045	30564193	68.70%	4.933%
17	12.663	1621	1628	1639	rVB	11759186	16006000	35.98%	2.583%
18	13.110	1696	1704	1712	rVB	12424317	17966501	40.39%	2.900%
19	14.051	1856	1864	1871	rBV	6248317	8783995	19.74%	1.418%
20	14.204	1881	1890	1897	rBV	19141486	26806654	60.26%	4.326%
21	14.374	1911	1919	1930	rBV	5619732	8211113	18.46%	1.325%
22	14.480	1930	1937	1942	rVV	2670257	3824486	8.60%	0.617%
23	14.545	1942	1948	1956	rVB	2555413	3757213	8.45%	0.606%
24	14.833	1991	1997	2000	rVV	4937682	6267138	14.09%	1.011%
25	14.880	2000	2005	2013	rVB	6842755	9701180	21.81%	1.566%
26	15.304	2069	2077	2088	rBV	11176776	13769731	30.95%	2.222%
27	15.527	2107	2115	2122	rBV	30276038	44487647	100.00%	7.180%
28	15.733	2143	2150	2155	rBV	18440219	23462811	52.74%	3.787%
29	15.962	2181	2189	2204	rBV	6573396	9012052	20.26%	1.454%
30	16.527	2278	2285	2293	rBV	16250205	22252866	50.02%	3.591%
31	17.215	2391	2402	2412	rBV	2905746	4135224	9.30%	0.667%
32	17.351	2417	2425	2439	rBV	19399550	26667067	59.94%	4.304%
33	19.621	2805	2811	2818	rBV	5503724	7022765	15.79%	1.133%
34	19.833	2841	2847	2859	rBV	24208781	27410688	61.61%	4.424%
35	21.362	3101	3107	3114	rBV	17117456	21448246	48.21%	3.462%
36	21.444	3115	3121	3124	rVV2	2414137	4265336	9.59%	0.688%

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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

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37	21.492	3124	3129	3145	rVB	25457918	35951598	80.81%	5.802%
38	22.421	3282	3287	3293	rVB	316909	534181	1.20%	0.086%
39	22.509	3295	3302	3324	rVV	18489991	28825296	64.79%	4.652%
40	23.515	3464	3473	3478	rBV	4849820	10442262	23.47%	1.685%
41	23.586	3478	3485	3492	rVB	8644677	16933678	38.06%	2.733%
42	24.333	3602	3612	3624	rBV	6233168	14993993	33.70%	2.420%
43	24.468	3627	3635	3644	rVV	1461379	3767252	8.47%	0.608%
44	24.550	3645	3649	3663	rVB3	246947	585087	1.32%	0.094%
45	27.926	4204	4223	4226	rBV2	5110895	20078911	45.13%	3.241%
46	28.973	4385	4401	4421	rVB2	3133443	13195850	29.66%	2.130%

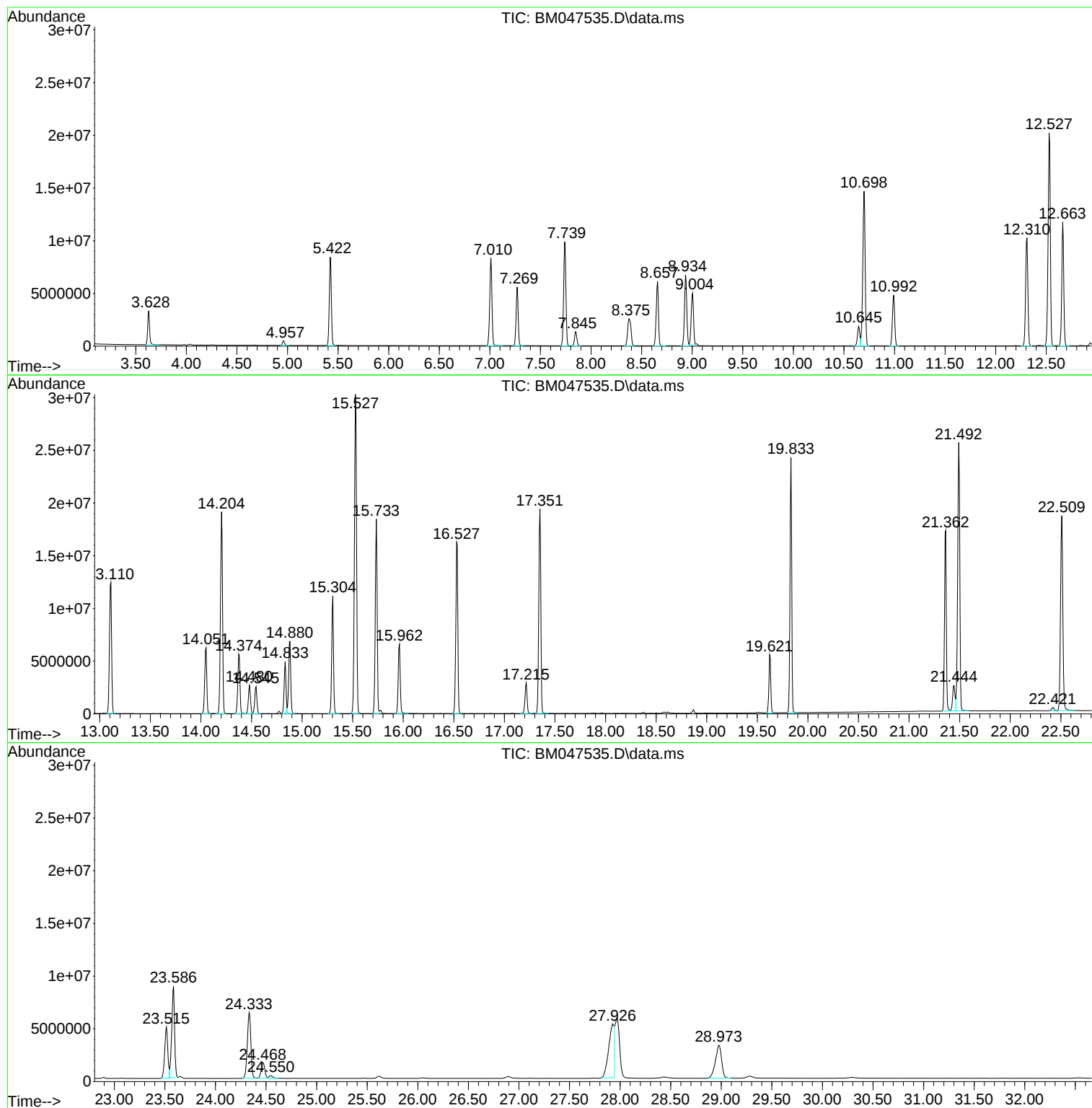
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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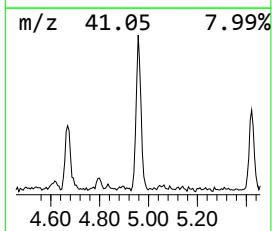
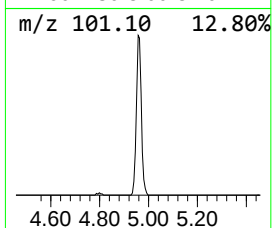
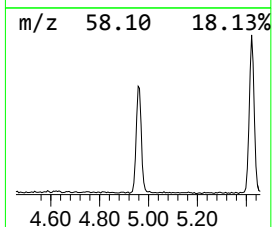
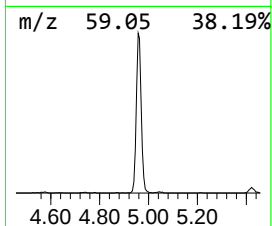
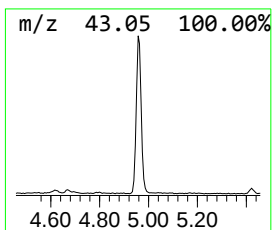
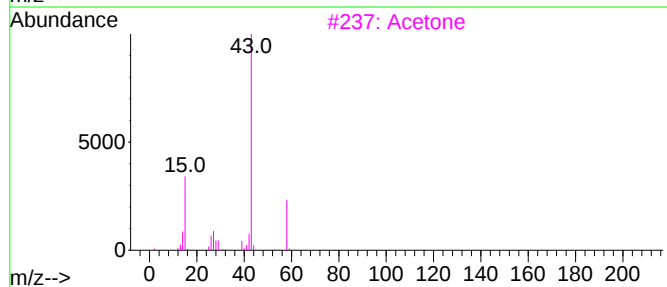
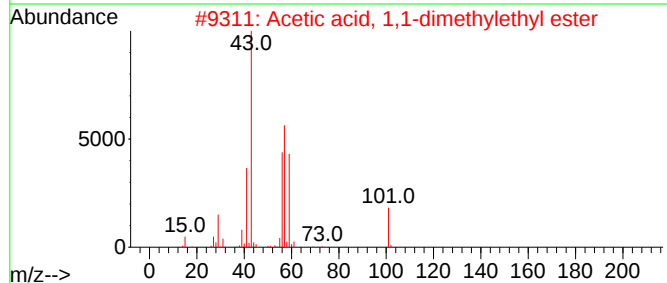
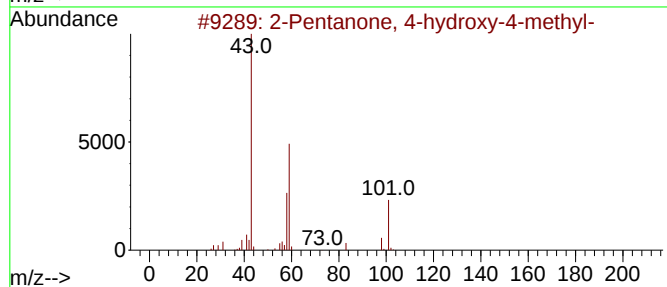
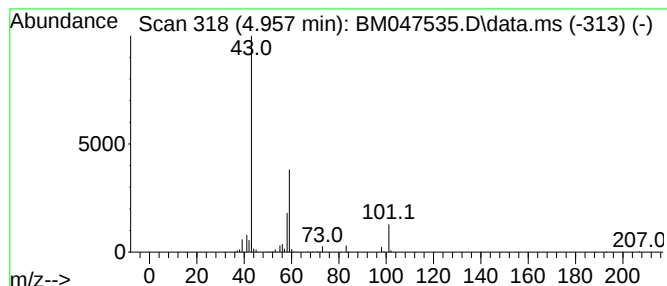
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	6.00 ng	643242	1,4-Dichlorobenzene-d4	7.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45		
3	Acetone	58	C3H6O	000067-64-1	9		
4	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9		
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9		



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Instrument :
BNA_M
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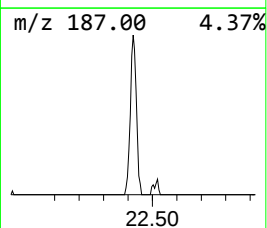
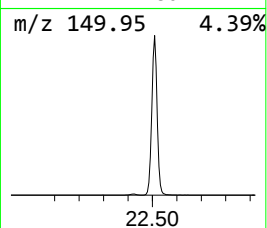
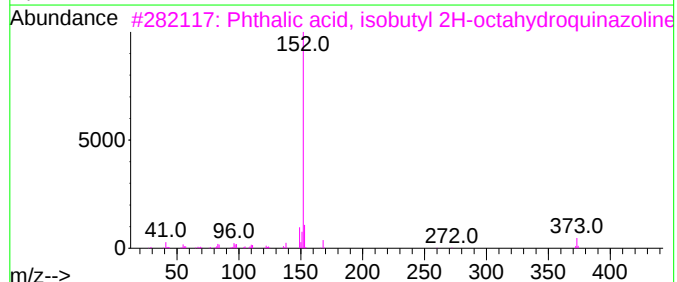
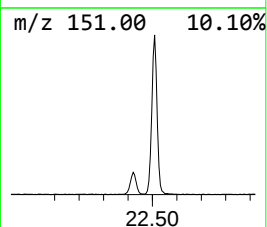
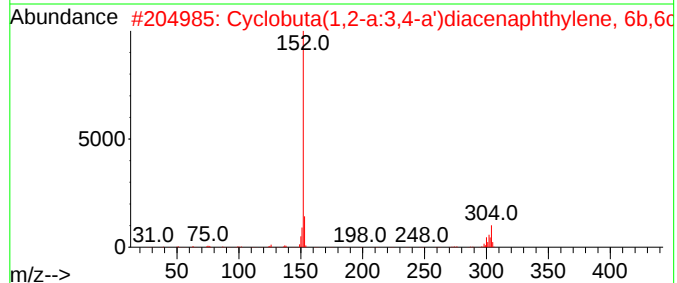
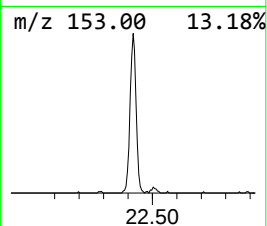
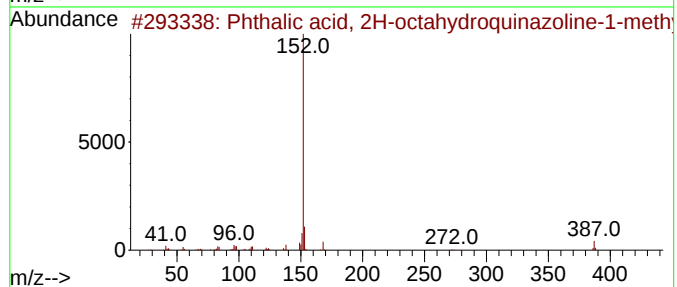
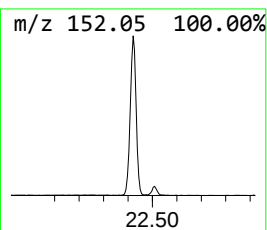
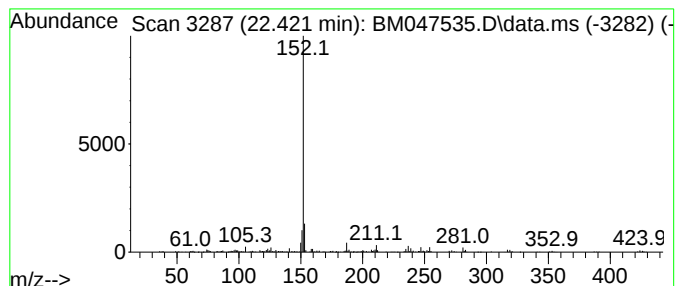
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Peak Number 2 Phthalic acid, 2H-octahydro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.421	2.50 ng	534181	Chrysene-d12	21.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2H-octahydroquina...	387	C23H33NO4	1000322-80-5	72
2			Cyclobuta(1,2-a:3,4-a')diacenaph...	304	C24H16	007259-03-2	72
3			Phthalic acid, isobutyl 2H-octah...	373	C22H31NO4	1000322-80-3	56
4			Phthalic acid, butyl 2H-octahydr...	373	C22H31NO4	1010322-80-4	56
5			(8R)-5-Allyl-8-ethyloctahydroind...	193	C13H23N	875587-44-3	45



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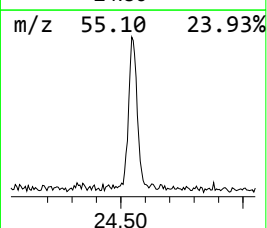
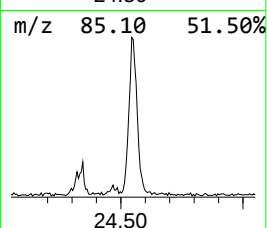
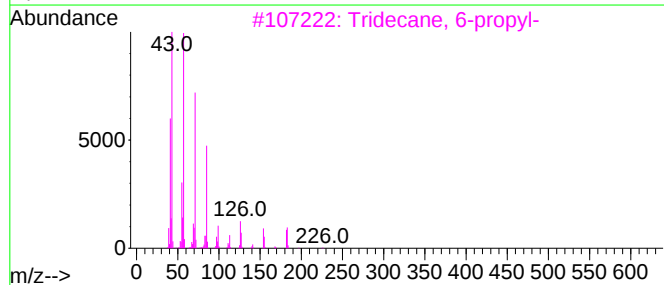
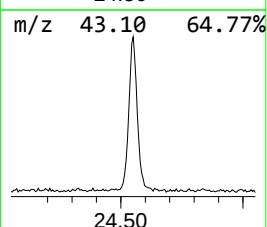
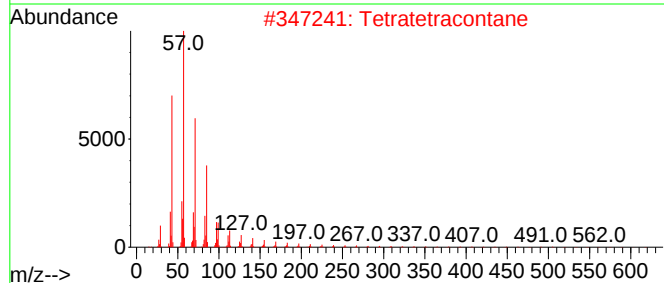
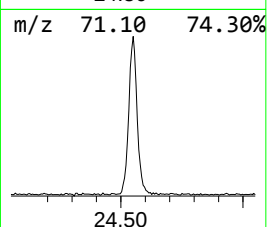
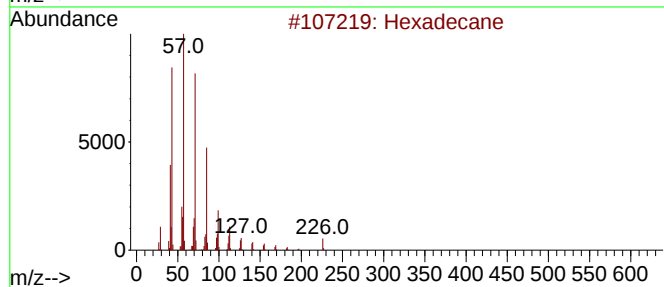
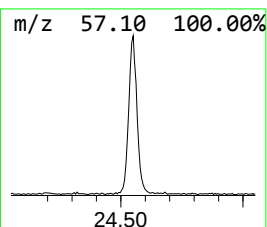
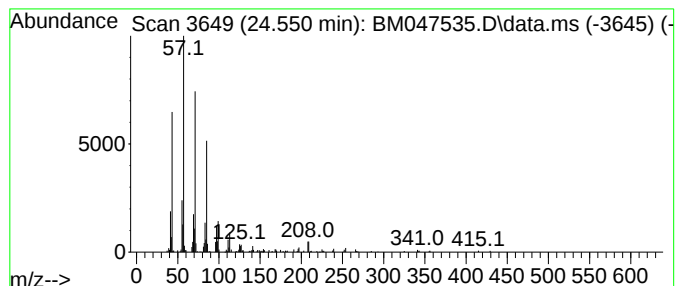
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Peak Number 3 Hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.550	3.11 ng	585087	Perylene-d12	24.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	6.0	ng	643242	1	7.851	2145190	20.0
Phthalic acid, ...	22.421	2.5	ng	534181	5	21.445	4265340	20.0
Hexadecane	24.550	3.1	ng	585087	6	24.474	3767250	20.0