

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011724\
 Data File : BG060343.D
 Acq On : 17 Jan 2024 15:01
 Operator : MA/JU
 Sample : PB158472BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB158472BL

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_G\Methods\8270-BG010824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.506	402	411	426	rBV	4505363	7019465	27.63%	6.758%
2	7.098	671	682	697	rBV	4468621	7754842	30.53%	7.466%
3	7.932	816	824	838	rBV	738813	1291938	5.09%	1.244%
4	9.095	1014	1022	1039	rBV	2920055	5291946	20.83%	5.095%
5	10.735	1293	1301	1311	rBV	1156440	2049335	8.07%	1.973%
6	13.191	1712	1719	1739	rBV	9015102	14482820	57.02%	13.943%
7	14.566	1946	1953	1963	rBV	2293991	3647267	14.36%	3.511%
8	16.058	2198	2207	2230	rBV	7862743	11934038	46.98%	11.489%
9	17.315	2414	2421	2435	rBV	3540980	5428290	21.37%	5.226%
10	19.624	2808	2814	2821	rVB2	208811	281191	1.11%	0.271%
11	19.936	2860	2867	2886	rBV	17836137	25401524	100.00%	24.455%
12	21.575	3139	3146	3160	rBV2	3698226	6277443	24.71%	6.044%
13	23.038	3387	3395	3402	rBV2	263511	534089	2.10%	0.514%
14	23.831	3522	3530	3538	rBV	339552	717556	2.82%	0.691%
15	24.742	3674	3685	3701	rBV	2487855	7389570	29.09%	7.114%
16	25.864	3867	3876	3890	rVB2	381172	1189204	4.68%	1.145%
17	27.198	4092	4103	4116	rBV3	348346	1247065	4.91%	1.201%
18	28.790	4364	4374	4391	rVB5	216629	933543	3.68%	0.899%
19	30.752	4691	4708	4714	rBV8	199580	998822	3.93%	0.962%

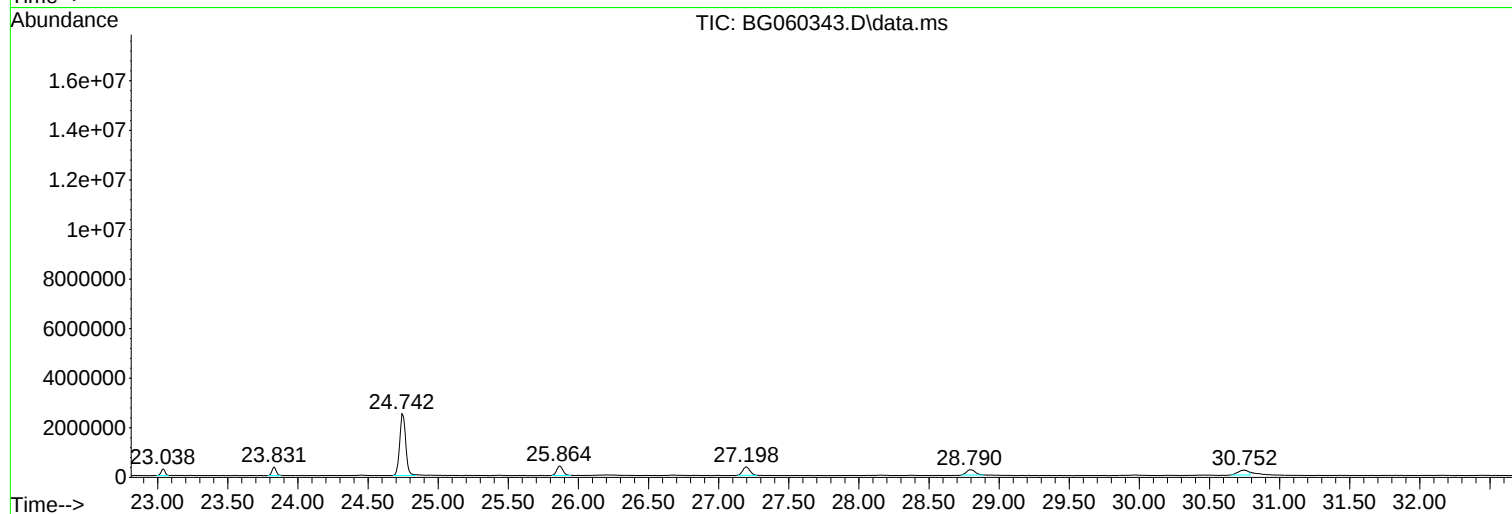
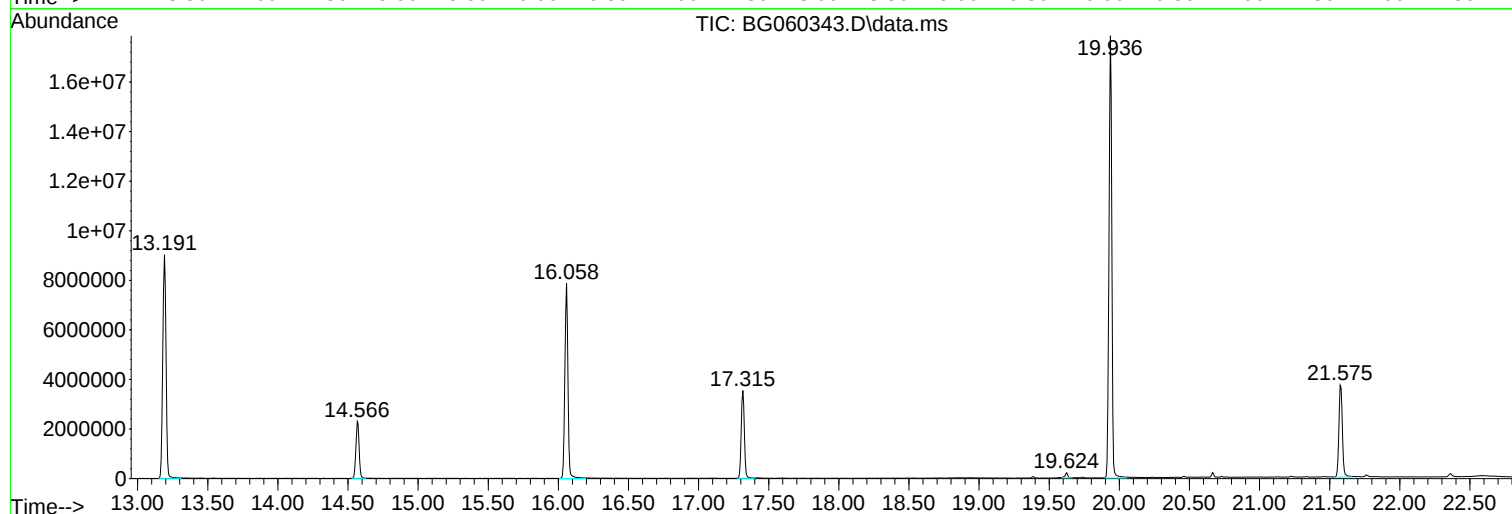
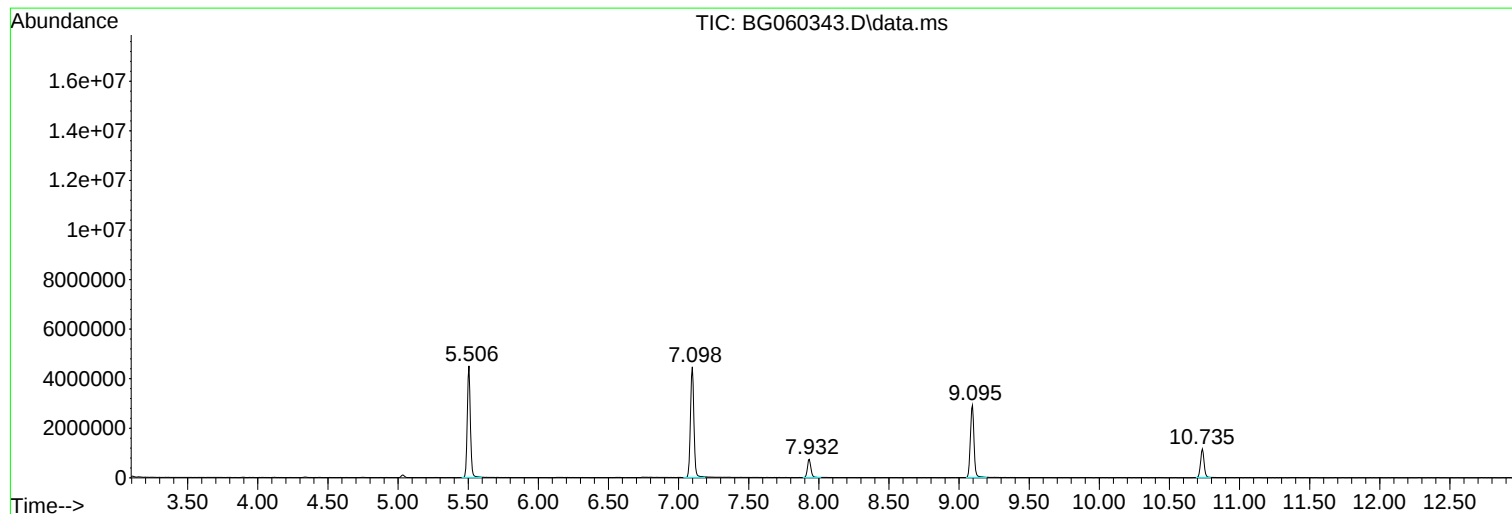
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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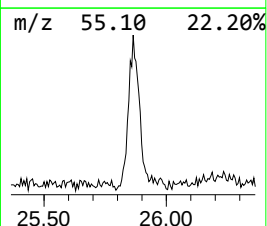
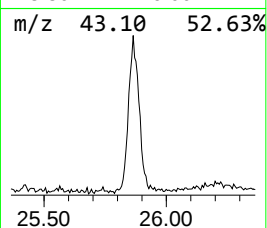
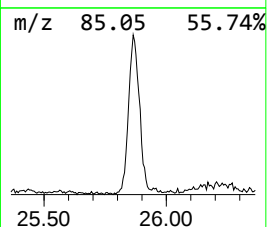
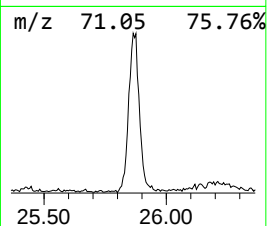
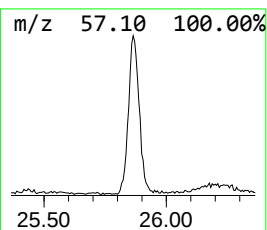
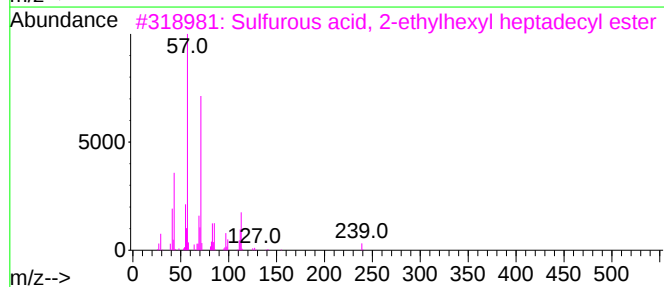
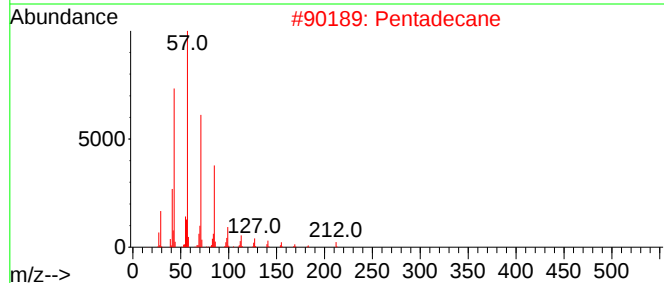
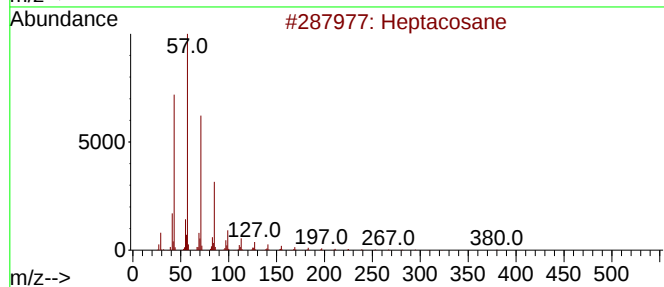
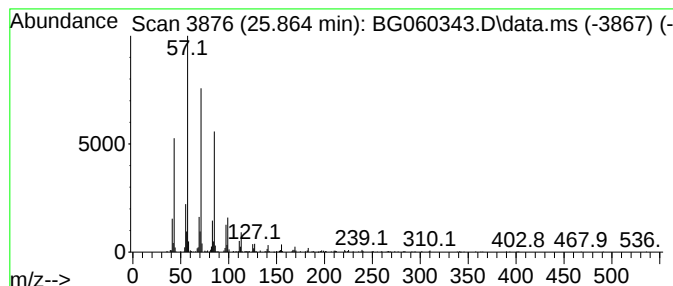
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.864	3.22 ng	1189200	Perylene-d12	24.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Pentadecane	212	C15H32	000629-62-9	80
3			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	58
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	58
5			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	58



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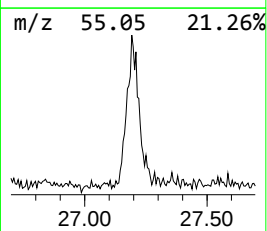
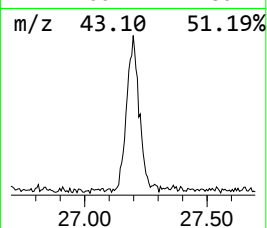
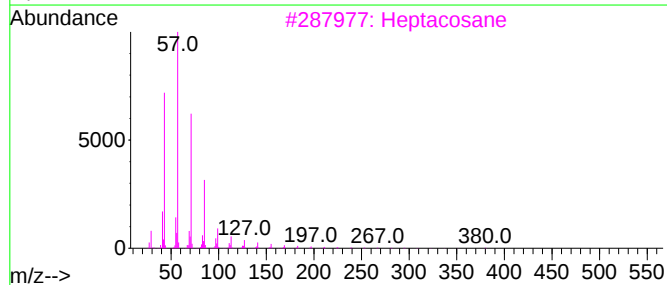
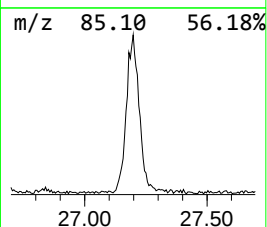
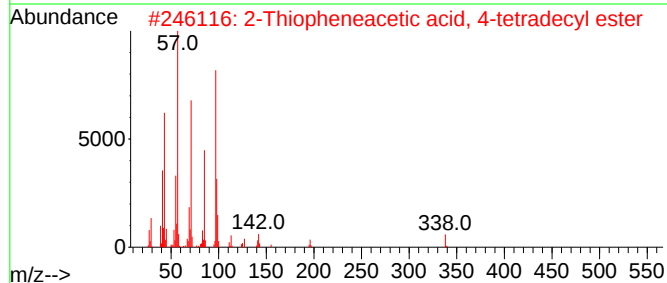
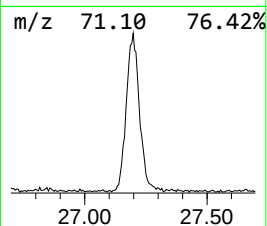
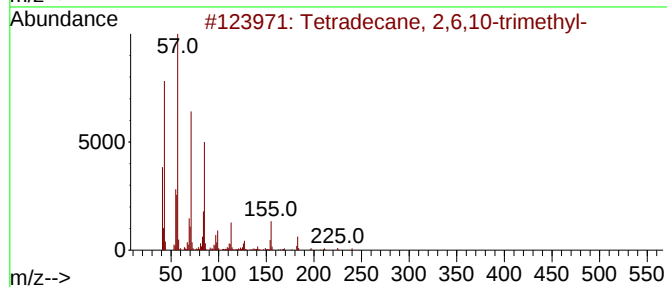
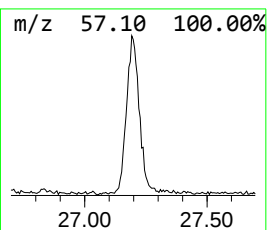
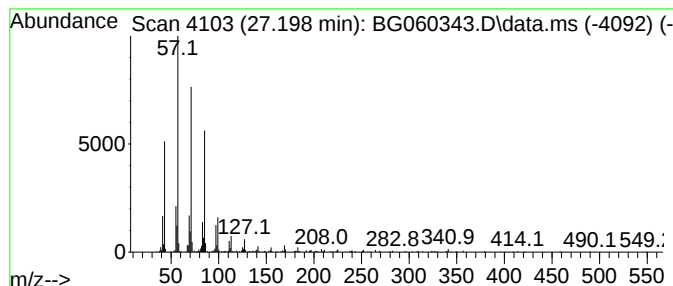
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tetradecane, 2,6,10-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.198	3.38 ng	1247070	Perylene-d12	24.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
2			2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1010280-67-0	80
3			Heptacosane	380	C27H56	000593-49-7	64
4			Docosane, 9-octyl-	422	C30H62	055319-83-0	60
5			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	58



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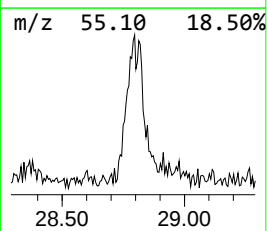
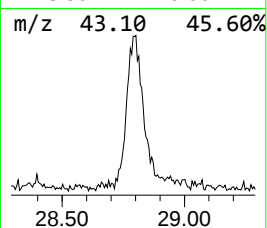
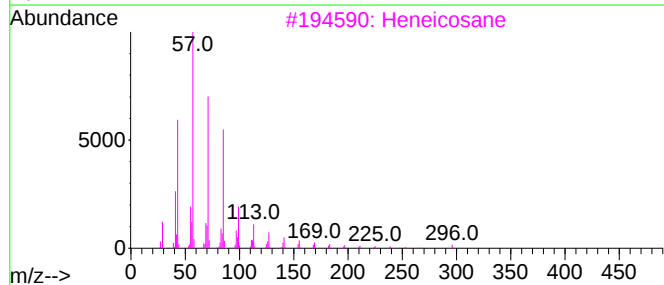
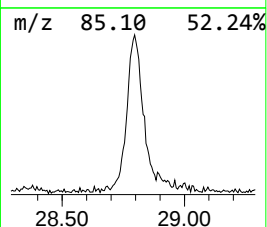
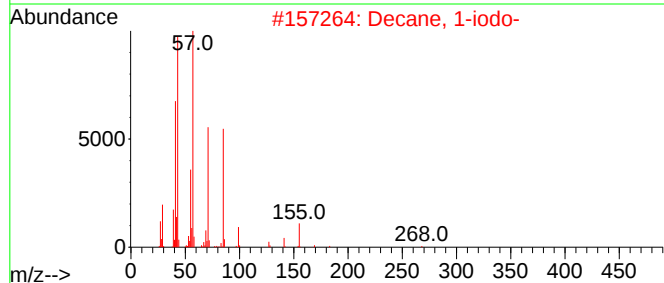
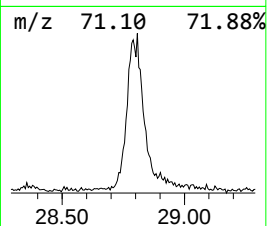
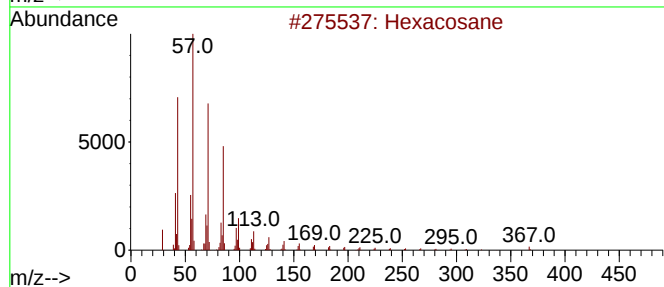
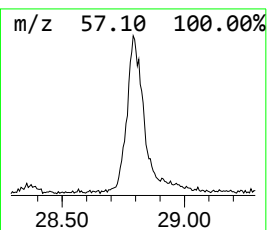
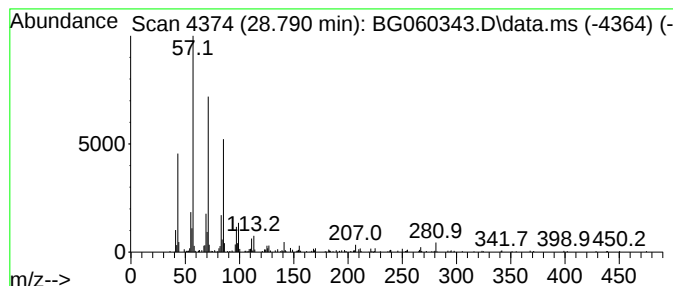
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Peak Number 3 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.790	2.53 ng	933543	Perylene-d12	24.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	83
2			Decane, 1-iodo-	268	C10H21I	002050-77-3	81
3			Heneicosane	296	C21H44	000629-94-7	80
4			Nonadecane	268	C19H40	000629-92-5	80
5			Tetracosane	338	C24H50	000646-31-1	80



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Misc :
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ClientSampleId :
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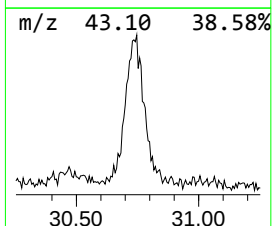
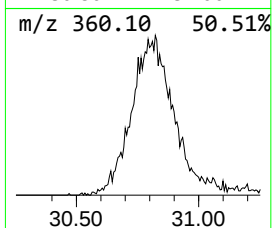
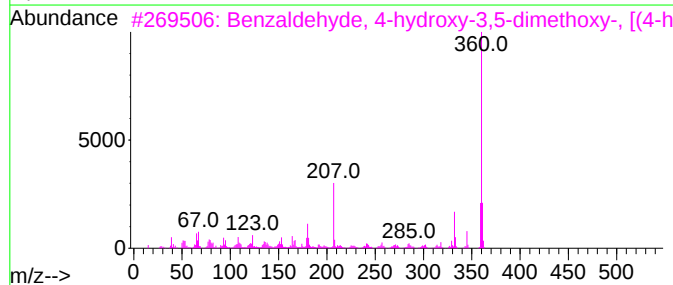
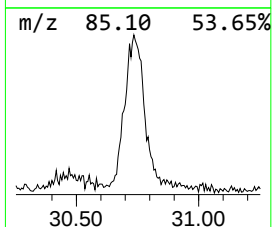
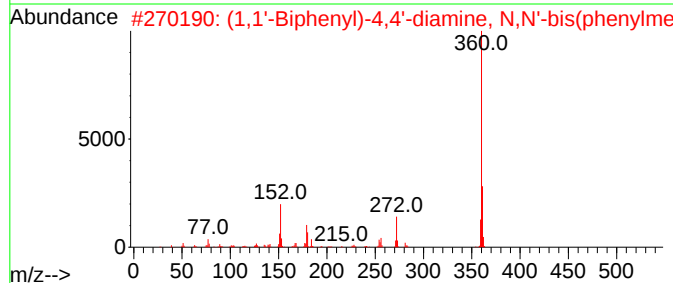
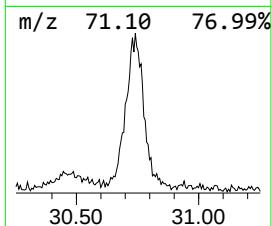
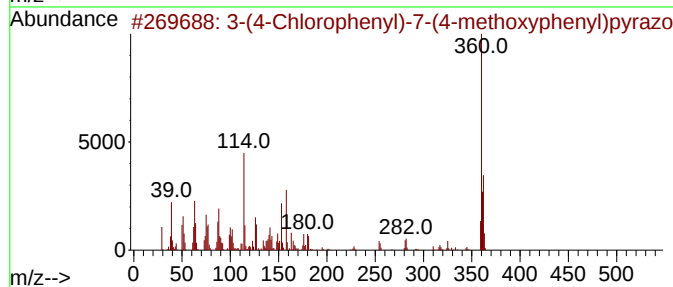
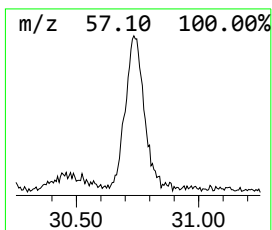
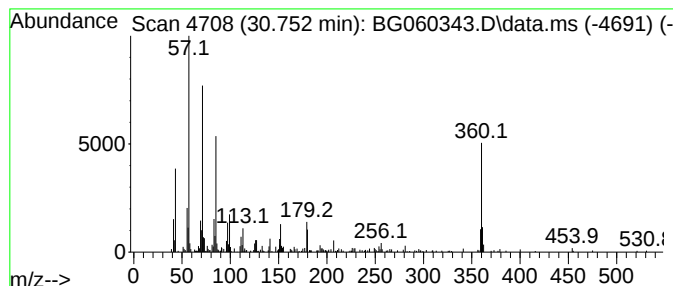
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown30.752 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.752	2.70 ng	998822	Perylene-d12	24.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(4-Chlorophenyl)-7-(4-methoxyphenyl)pyrazole	360	C20H13ClN4O	1000460-08-0	18		
2	(1,1'-Biphenyl)-4,4'-diamine, N,N'-bis(phenylmethyl)-	360	C26H20N2	006311-48-4	18		
3	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-, [(4-hydroxy-3,5-dimethoxyphenyl)methyl]-	360	C18H20N2O6	014414-32-5	14		
4	1,10-Phenanthroline, 2,9-dimethyl-, N,N'-bis(phenylmethyl)-	360	C26H20N2	004733-39-5	14		
5	Bis-(4-(2,5-dioxo-2,5-dihydropyrrolo[2,1-b]oxazol-6-yl)phenyl)-	360	C20H12N2O5	013132-94-0	11		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptacosane	25.864	3.2	ng	1189200	6	24.742	7389570	20.0
Tetradecane, 2,...	27.198	3.4	ng	1247070	6	24.742	7389570	20.0
Hexacosane	28.790	2.5	ng	933543	6	24.742	7389570	20.0
unknown30.752	30.752	2.7	ng	998822	6	24.742	7389570	20.0