

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
 Data File : BG056360.D
 Acq On : 19 Jan 2023 23:55
 Operator : CG/JU
 Sample : 01172-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-F

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056360.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.317	3	5	17	rVB	116960	154326	7.08%	1.274%
2	5.344	344	350	362	rVB	112496	185169	8.50%	1.529%
3	5.826	425	432	443	rBV	500637	838028	38.45%	6.921%
4	7.447	700	708	721	rBV	510702	894948	41.06%	7.391%
5	8.305	847	854	861	rBV	169046	282830	12.98%	2.336%
6	9.480	1044	1054	1065	rBB	303330	546176	25.06%	4.511%
7	11.137	1328	1336	1344	rBV	215498	392669	18.01%	3.243%
8	13.546	1737	1746	1756	rBV	1147463	1704510	78.20%	14.077%
9	14.921	1971	1980	1986	rVB	388680	593288	27.22%	4.900%
10	16.255	2202	2207	2214	rVB2	34812	55400	2.54%	0.458%
11	16.401	2224	2232	2238	rBV	731229	1145052	52.53%	9.456%
12	17.659	2439	2446	2450	rBV	439105	719814	33.02%	5.945%
13	17.700	2450	2453	2460	rVB	120515	169322	7.77%	1.398%
14	17.788	2464	2468	2473	rBV	29375	42674	1.96%	0.352%
15	18.499	2585	2589	2597	rBV3	90334	166774	7.65%	1.377%
16	18.570	2598	2601	2607	rVB2	30766	49210	2.26%	0.406%
17	18.722	2621	2627	2631	rBV3	33699	80178	3.68%	0.662%
18	19.692	2787	2792	2797	rBV	324743	448005	20.55%	3.700%
19	20.021	2844	2848	2849	rBV2	33804	50820	2.33%	0.420%
20	20.050	2849	2853	2860	rVB	299556	427271	19.60%	3.529%
21	20.232	2879	2884	2890	rVB	1759555	2179717	100.00%	18.001%
22	21.954	3169	3177	3182	rBV3	441427	982612	45.08%	8.115%

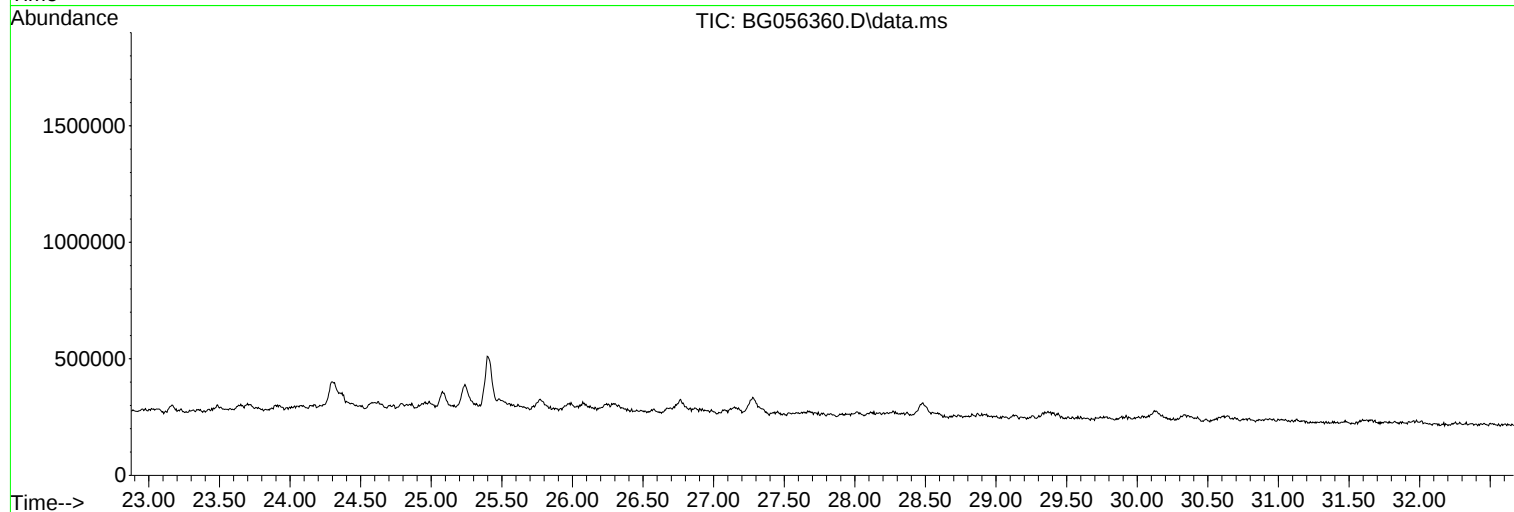
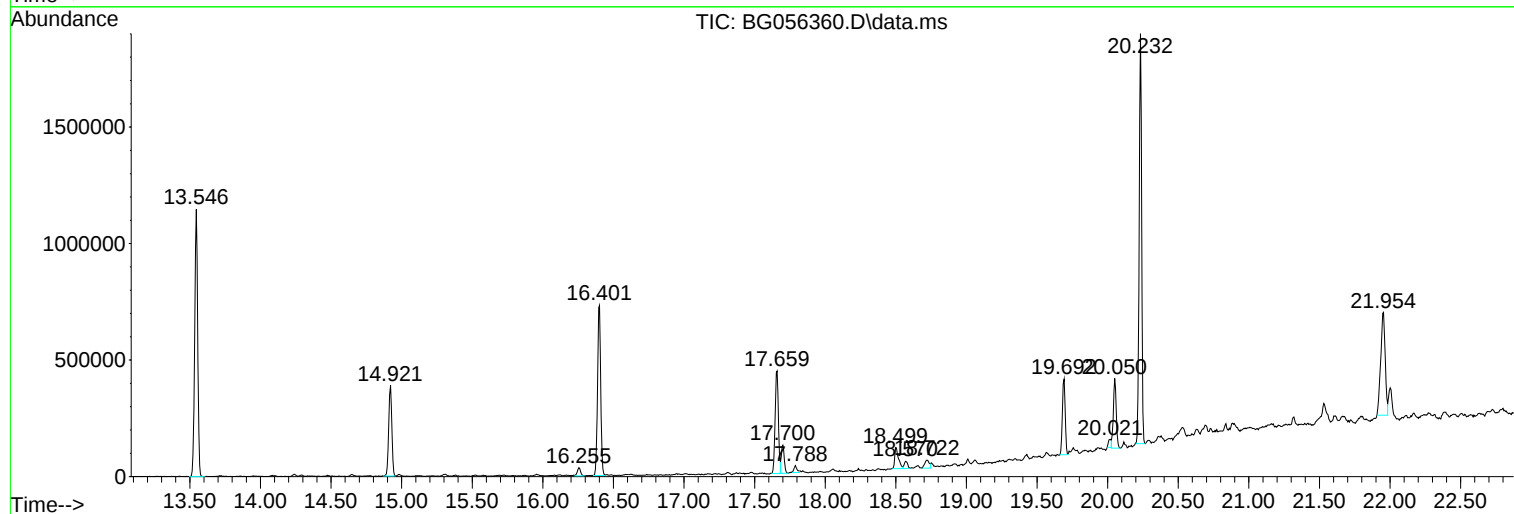
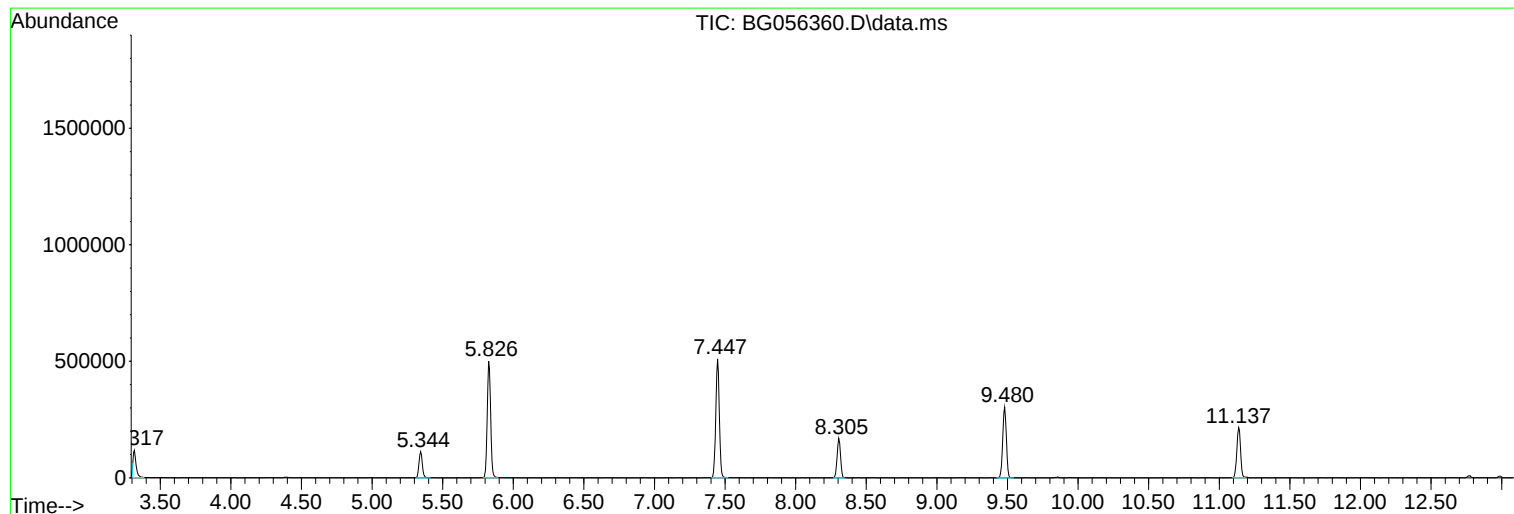
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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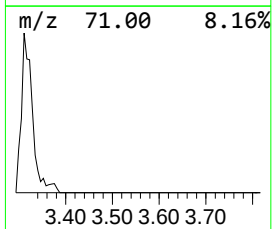
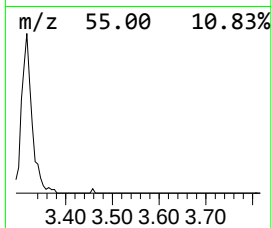
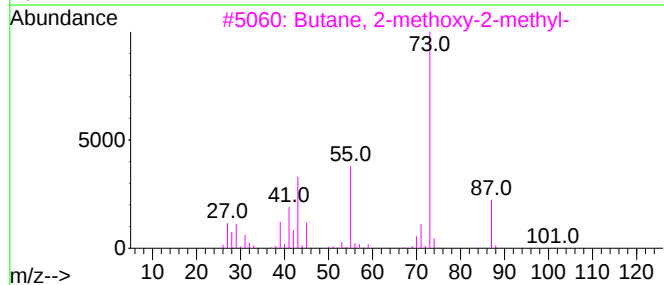
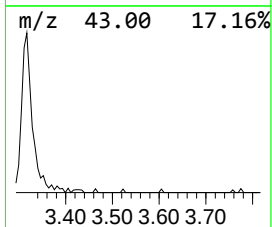
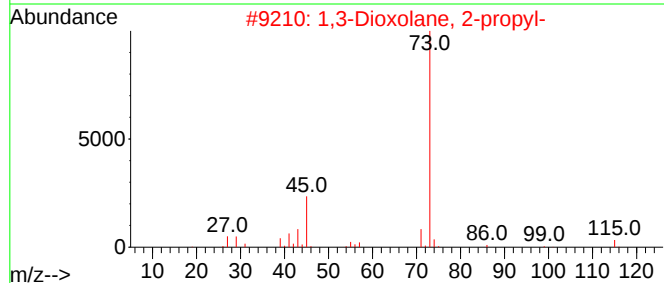
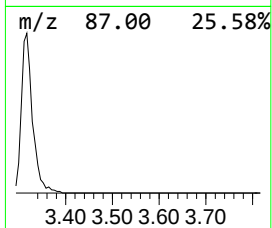
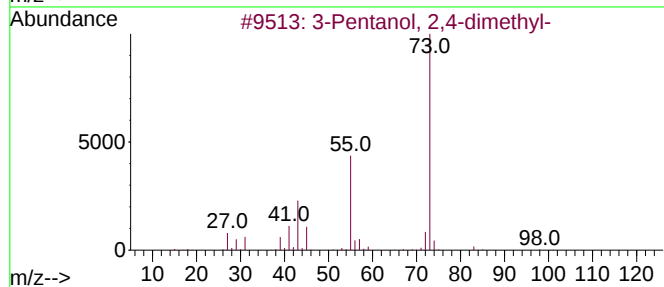
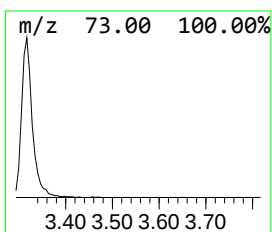
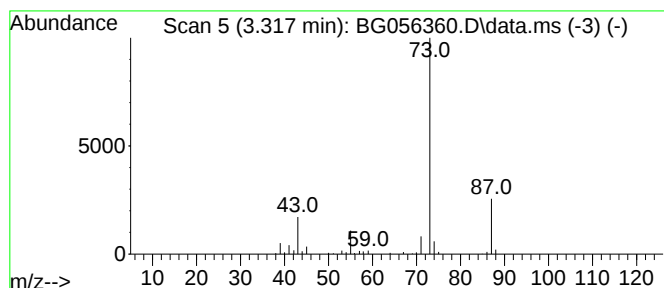
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.317 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.317	10.91 ng	154326	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
2			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
3			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
4			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5			2-Propanone, oxime	73	C3H7NO	000127-06-0	7



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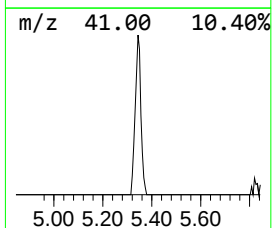
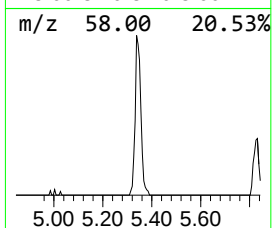
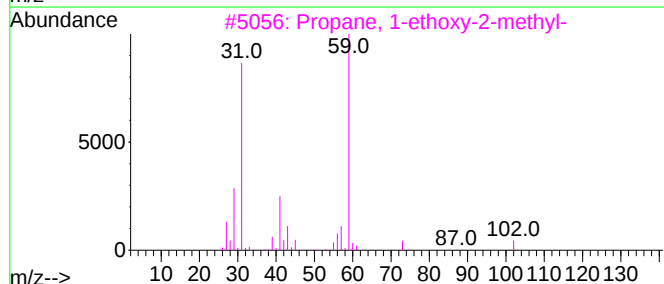
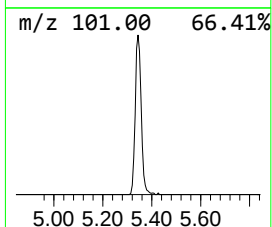
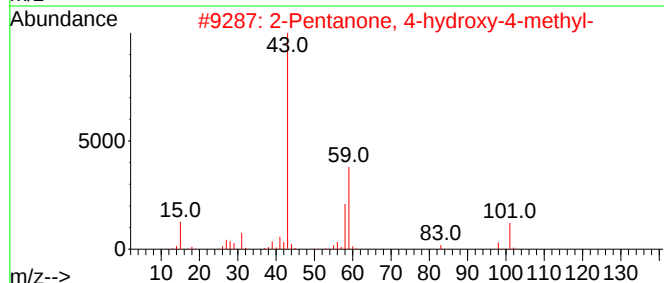
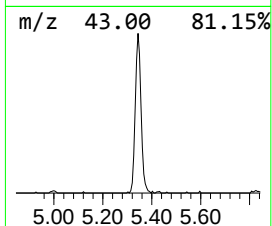
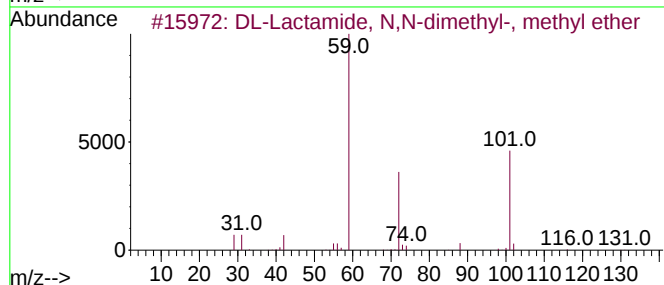
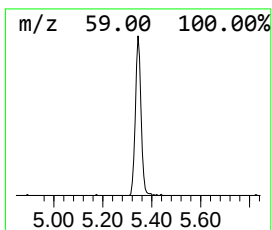
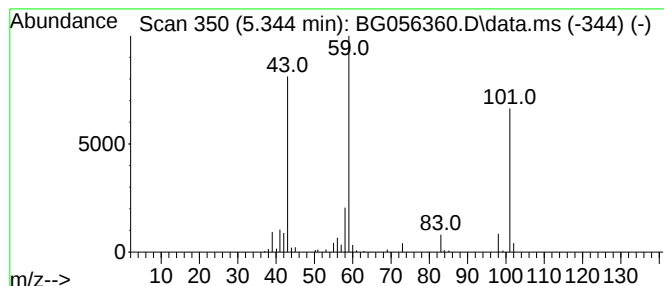
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.344 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.344	13.09 ng	185169	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	42
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
4			Guanidine	59	CH5N3	000113-00-8	37
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	35



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BNA_G
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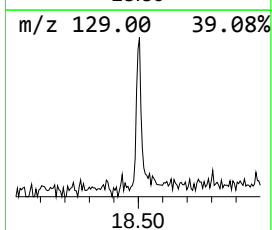
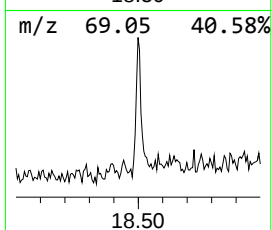
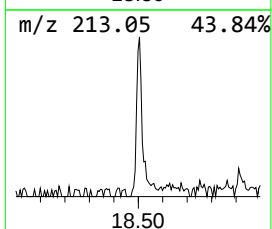
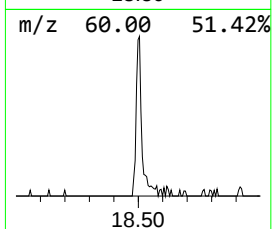
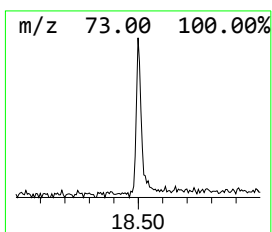
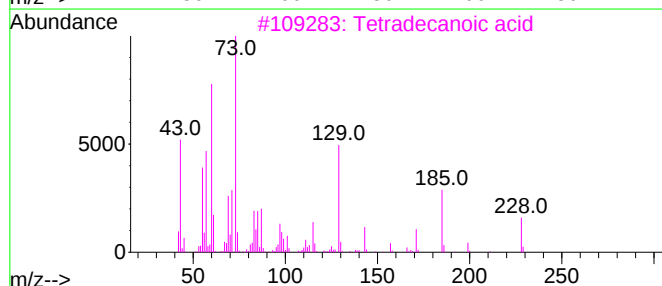
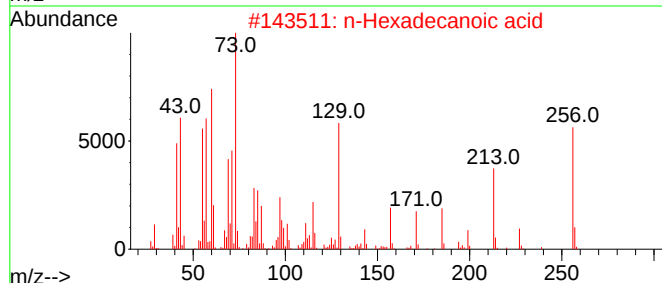
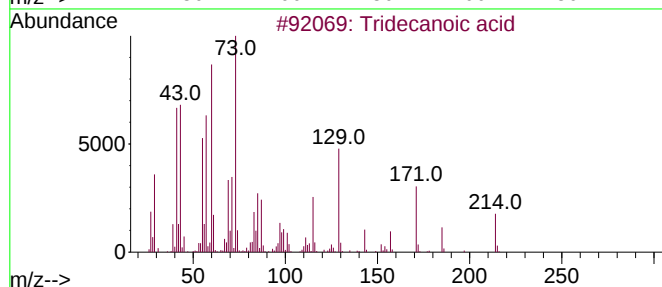
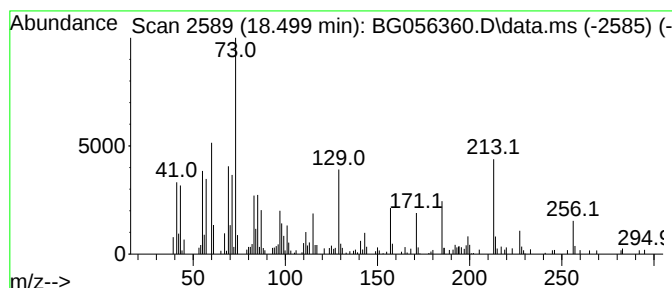
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Peak Number 3 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.499	4.63 ng	166774	Phenanthrene-d10	17.659

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Undecanoic acid	186	C11H22O2	000112-37-8	53
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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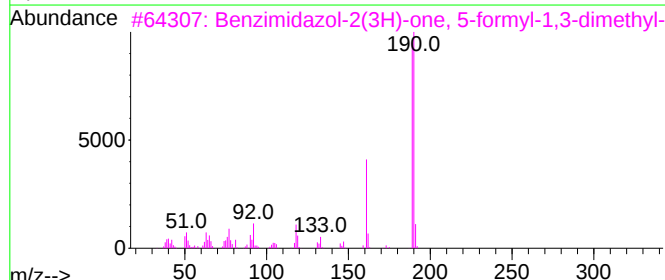
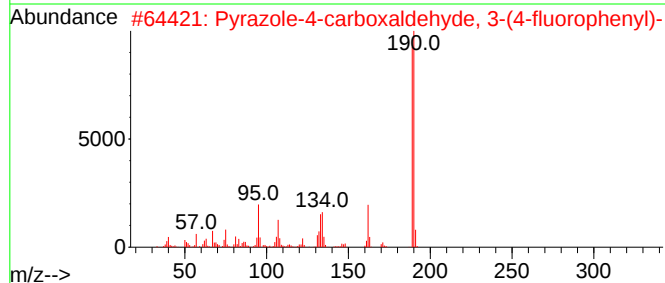
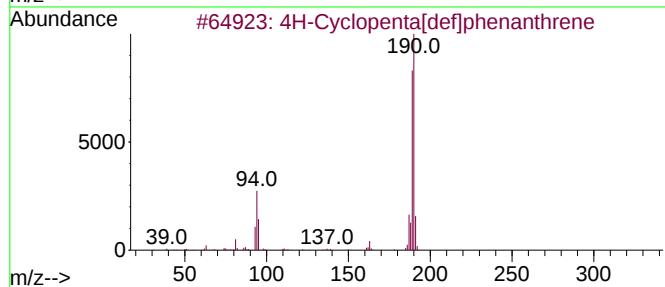
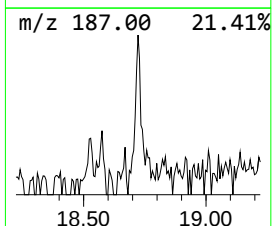
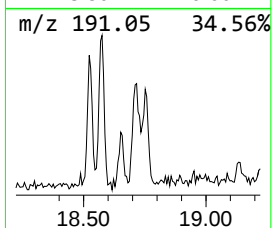
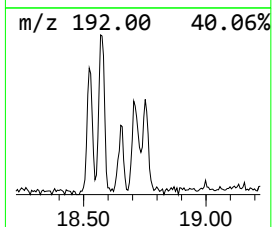
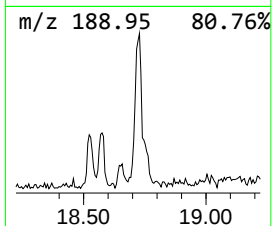
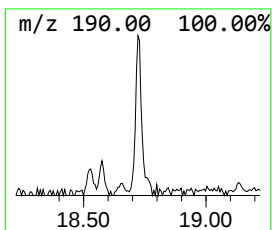
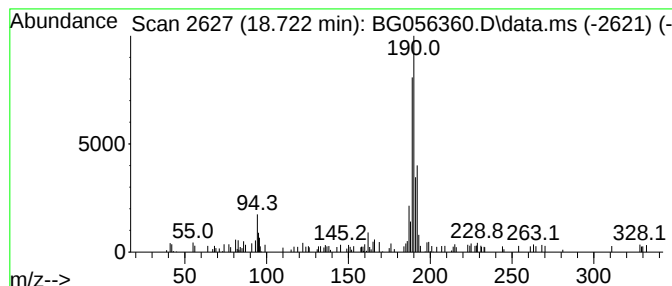
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Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.722	2.23 ng	80178	Phenanthrene-d10	17.659

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
2			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	47
3			Benzimidazol-2(3H)-one, 5-formyl...	190	C10H10N2O2	055241-49-1	38
4			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	30
5			6-(4-Fluorophenyl)-2-hydroxypyri...	231	C13H10FN02	1000509-20-7	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.317	3.317	10.9	ng	154326	1	8.305	282830	20.0
unknown5.344	5.344	13.1	ng	185169	1	8.305	282830	20.0
Tridecanoic acid	18.499	4.6	ng	166774	4	17.659	719814	20.0
4H-Cyclopenta[d...]	18.722	2.2	ng	80178	4	17.659	719814	20.0