

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059758.D
 Acq On : 18 Nov 2023 10:31
 Operator : MA/JU
 Sample : 05374-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RB21197

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.834	409	416	425	rVB2	282597	445006	20.94%	4.366%
2	7.461	686	693	699	rVB	334112	564062	26.55%	5.534%
3	8.342	836	843	850	rBV2	88118	162655	7.66%	1.596%
4	9.500	1033	1040	1042	rBV2	36350	61234	2.88%	0.601%
5	9.541	1042	1047	1053	rVB2	198829	361590	17.02%	3.548%
6	11.186	1319	1327	1334	rBV2	117690	228987	10.78%	2.247%
7	13.589	1730	1736	1744	rVB	957149	1429195	67.27%	14.022%
8	14.770	1932	1937	1941	rVB3	23652	33908	1.60%	0.333%
9	14.970	1965	1971	1977	rVB2	211409	340074	16.01%	3.336%
10	16.451	2216	2223	2233	rBV	803200	1189194	55.97%	11.667%
11	17.344	2367	2375	2380	rBV9	26478	62948	2.96%	0.618%
12	17.538	2405	2408	2414	rVB5	17891	31493	1.48%	0.309%
13	17.720	2433	2439	2443	rBV	362631	574729	27.05%	5.639%
14	17.761	2443	2446	2451	rVB2	111092	159942	7.53%	1.569%
15	17.849	2458	2461	2466	rVB3	22024	32114	1.51%	0.315%
16	18.119	2505	2507	2514	rVB5	21266	31336	1.47%	0.307%
17	18.531	2572	2577	2583	rBV4	142882	194528	9.16%	1.909%
18	18.578	2583	2585	2590	rVV6	18591	34223	1.61%	0.336%
19	18.630	2591	2594	2598	rVB6	24783	30920	1.46%	0.303%
20	18.713	2604	2608	2613	rBV7	13029	28277	1.33%	0.277%
21	18.783	2613	2620	2621	rBV7	19046	33124	1.56%	0.325%
22	19.124	2675	2678	2680	rBV4	17107	21679	1.02%	0.213%
23	19.753	2779	2785	2788	rBV	124623	174821	8.23%	1.715%
24	19.788	2788	2791	2798	rVB8	56879	87330	4.11%	0.857%
25	19.888	2804	2808	2811	rBV6	12629	21260	1.00%	0.209%
26	20.070	2835	2839	2840	rBV4	18710	22154	1.04%	0.217%
27	20.117	2843	2847	2851	rVB	74965	112302	5.29%	1.102%
28	20.293	2871	2877	2885	rBV	1720395	2124703	100.00%	20.846%
29	20.781	2958	2960	2963	rBV4	23424	25698	1.21%	0.252%
30	21.386	3059	3063	3068	rVB7	18702	31925	1.50%	0.313%
31	21.586	3091	3097	3102	rBV9	80234	139397	6.56%	1.368%
32	22.050	3169	3176	3181	rBV	299415	561847	26.44%	5.512%
33	22.097	3181	3184	3191	rVB4	44004	75500	3.55%	0.741%
34	23.137	3356	3361	3363	rBV6	21200	31224	1.47%	0.306%
35	23.249	3375	3380	3384	rBV7	35610	58966	2.78%	0.579%
36	23.372	3394	3401	3402	rBV6	16692	34749	1.64%	0.341%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.930	3493	3496	3499	rBV5	17714	26215	1.23%	0.257%
38	24.453	3582	3585	3587	rBV4	29082	36762	1.73%	0.361%
39	25.440	3749	3753	3754	rBV4	19267	22121	1.04%	0.217%
40	25.634	3776	3786	3794	rBV2	176616	554421	26.09%	5.439%

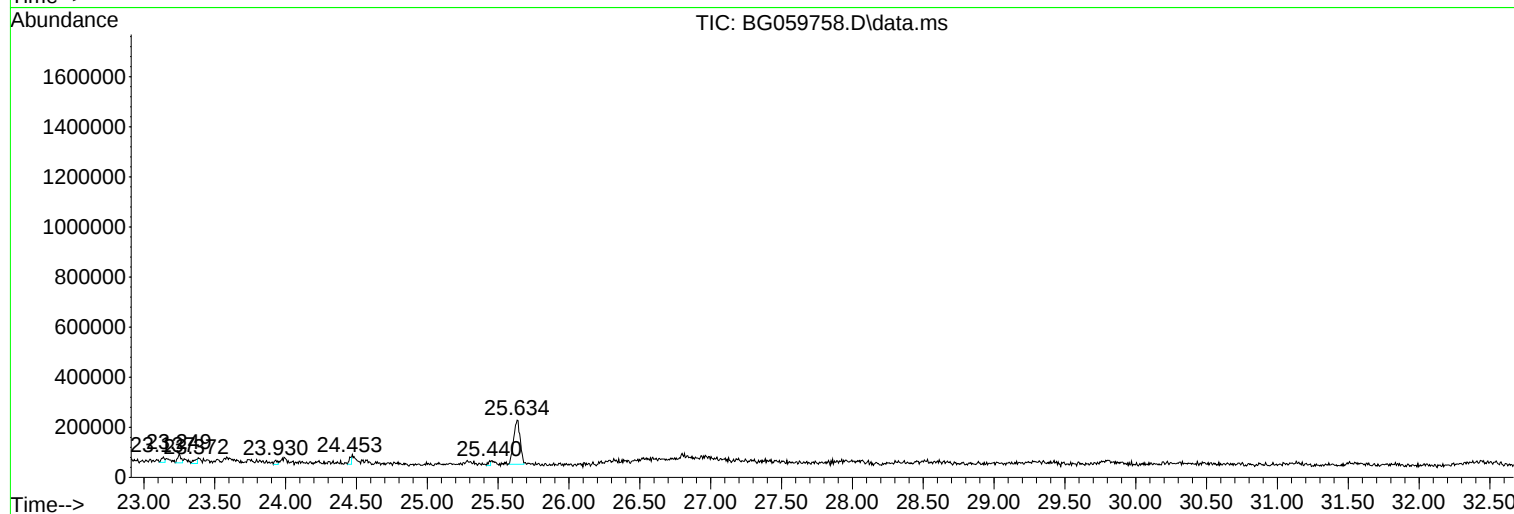
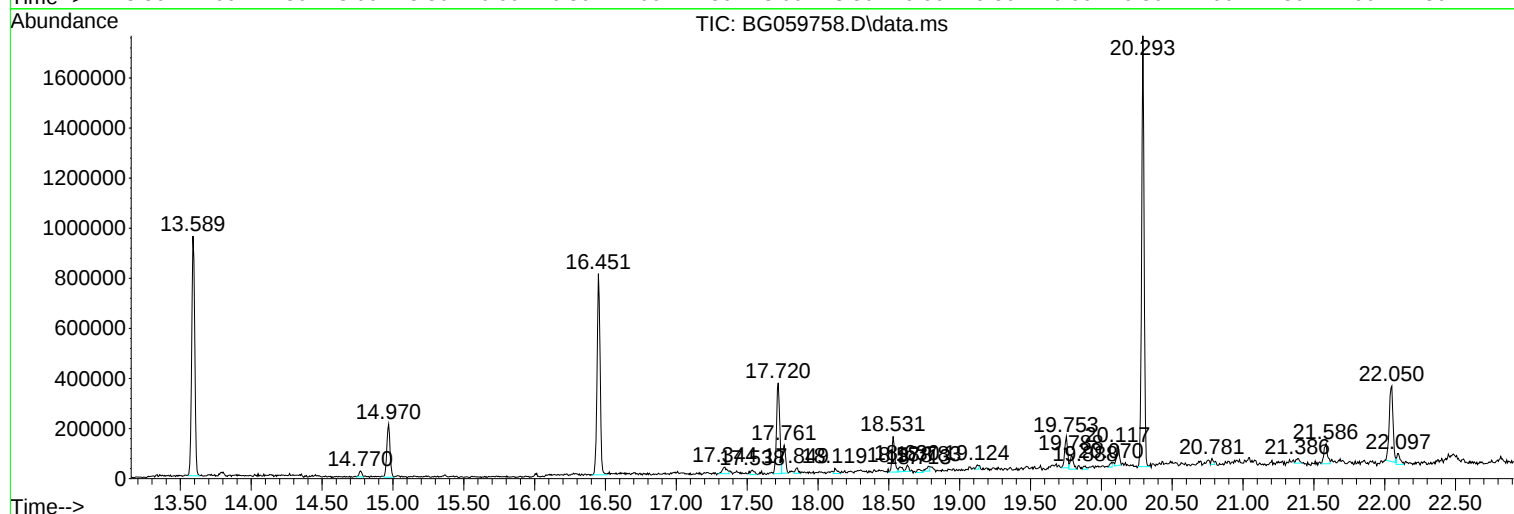
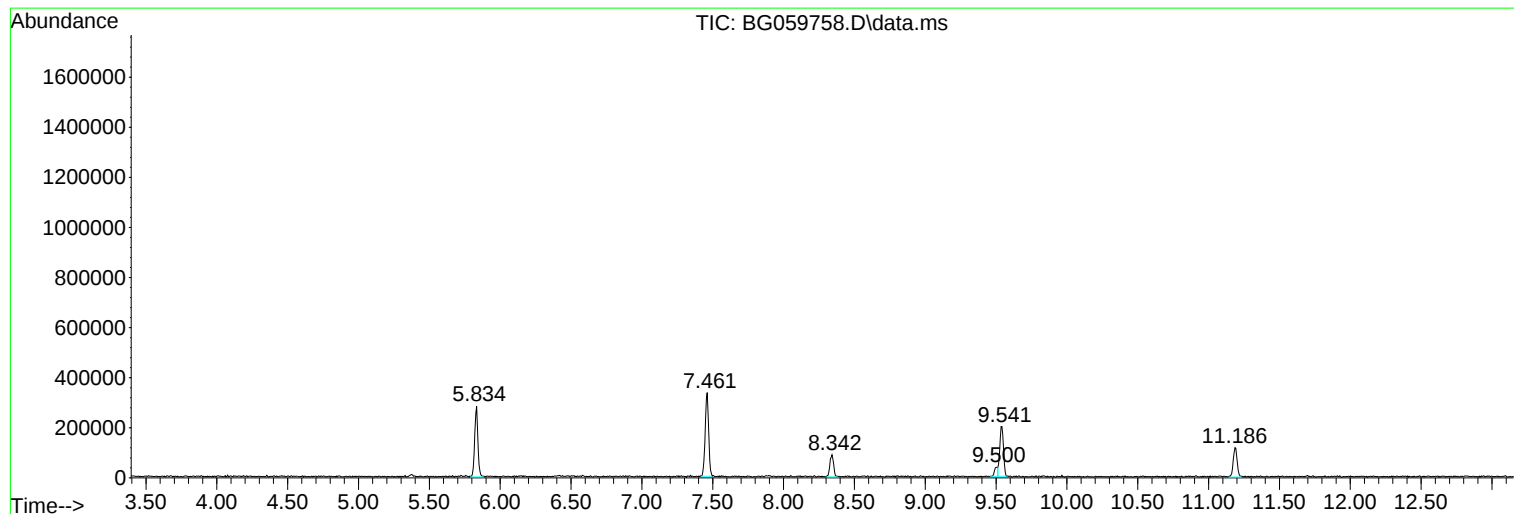
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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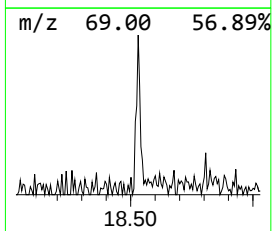
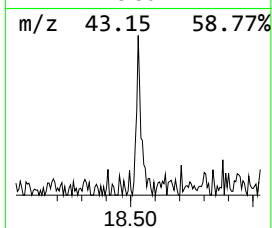
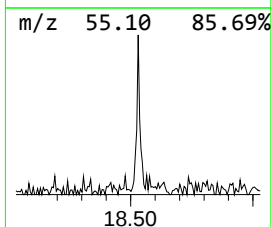
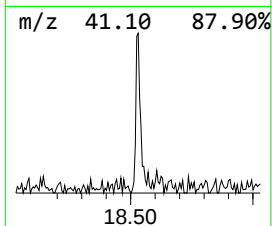
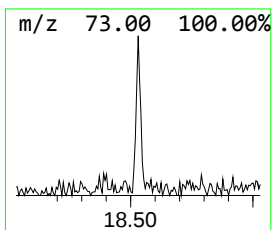
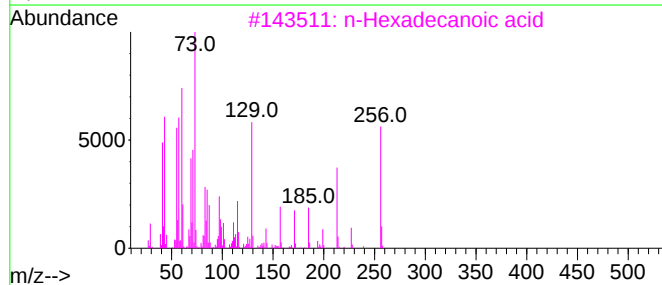
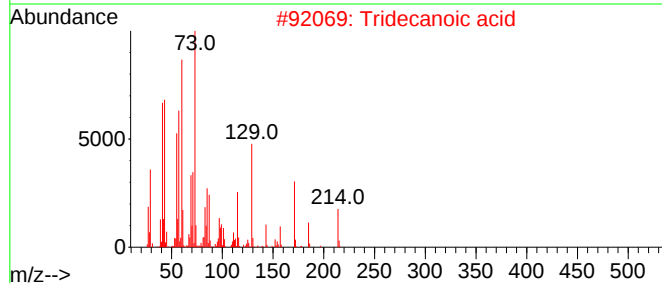
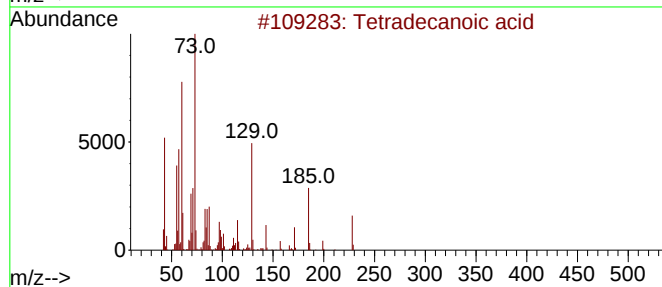
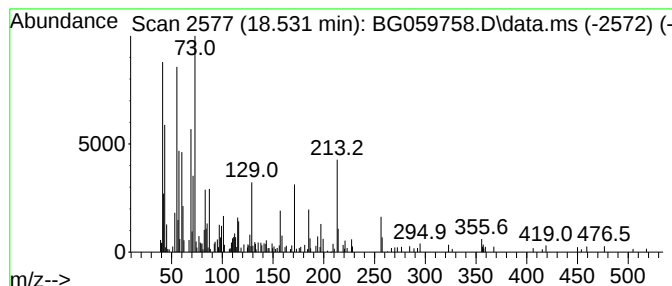
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown18.531 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.531	6.77 ng	194528	Phenanthrene-d10	17.720

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	45
2			Tridecanoic acid	214	C13H26O2	000638-53-9	43
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	27
5			n-Decanoic acid	172	C10H20O2	000334-48-5	27



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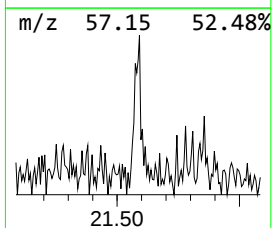
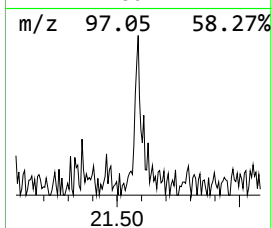
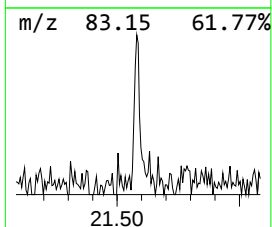
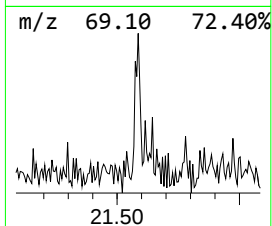
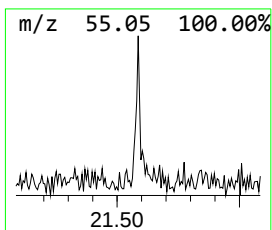
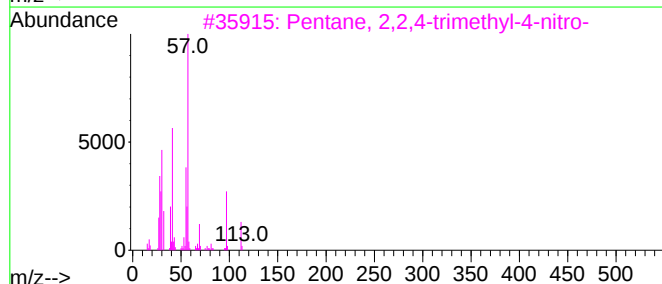
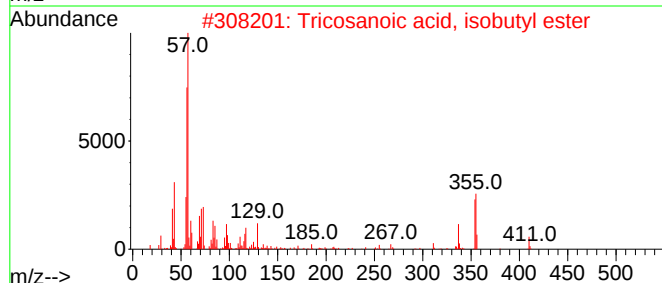
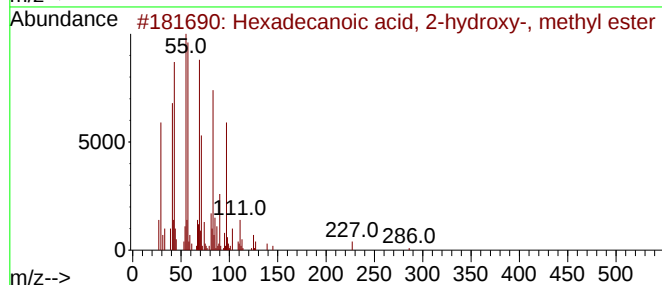
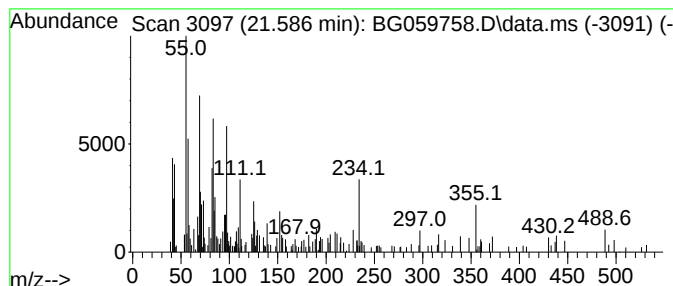
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown21.586 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.586	4.96 ng	139397	Chrysene-d12	22.050

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	10
2			Tricosanoic acid, isobutyl ester	410	C27H54O2	1000405-17-2	9
3			Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	9
4			Cyclopentanemethanamine, 2-amino-	114	C6H14N2	021544-02-5	9
5			9,19-Cyclolanostan-3-ol, 24,24-e...	498	C33H54O3	1000190-57-2	4



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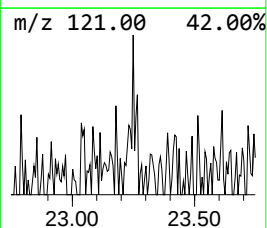
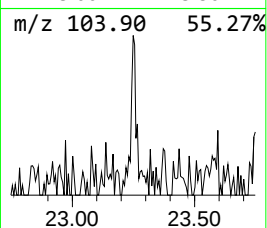
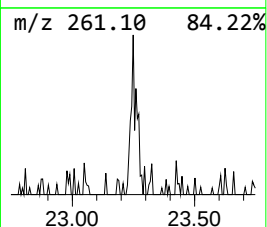
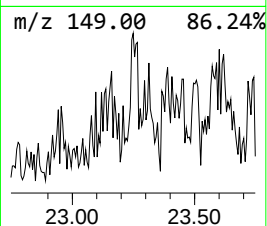
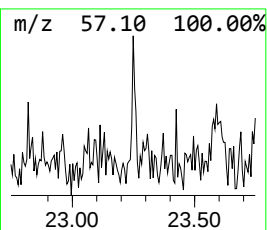
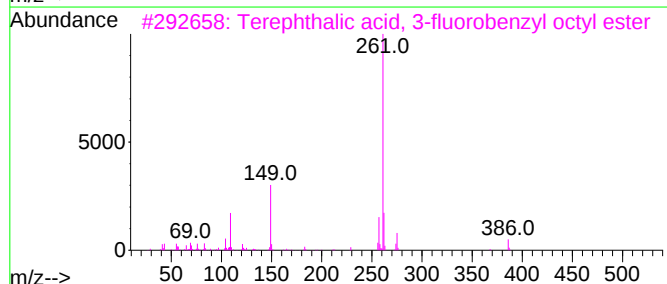
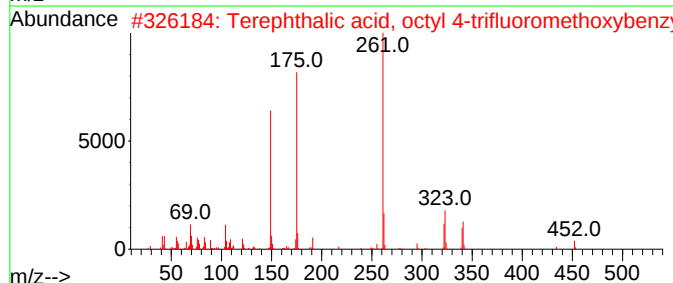
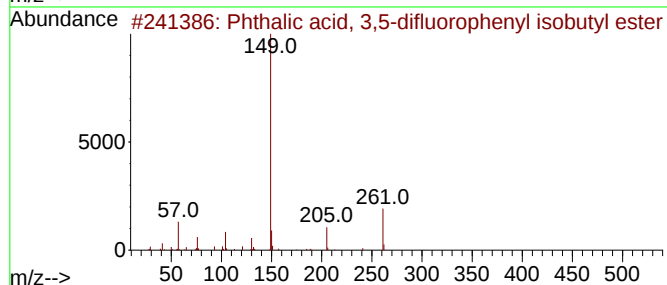
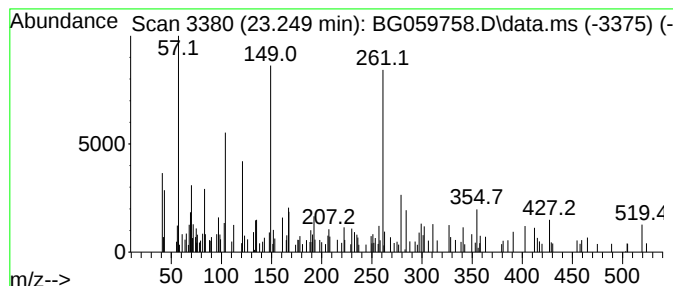
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phthalic acid, 3,5-difluoro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.249	2.10 ng	58966	Chrysene-d12	22.050

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 3,5-difluoropheny...	334	C18H16F2O4	1000314-97-0	53
2			Terephthalic acid, octyl 4-trifl...	452	C24H27F3O5	1000415-98-0	38
3			Terephthalic acid, 3-fluorobenzy...	386	C23H27F3O4	1000416-15-7	30
4			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	25
5			4-Acetyl-5-methyl-1-(3-nitrophen...	261	C12H11N3O4	1000443-31-2	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown18.531	18.531	6.8	ng	194528	4	17.720	574729	20.0
unknown21.586	21.586	5.0	ng	139397	5	22.050	561847	20.0
Phthalic acid, ...	23.249	2.1	ng	58966	5	22.050	561847	20.0