

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032122\
 Data File : BG052765.D
 Acq On : 21 Mar 2022 13:17
 Operator : CG/JU
 Sample : N1983-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 124042

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-BG031522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.702	386	394	404	rBV	911173	1499811	52.22%	8.161%
2	7.294	656	665	673	rBV	968779	1669023	58.11%	9.081%
3	8.146	803	810	817	rVB	185059	318399	11.09%	1.732%
4	9.303	996	1007	1016	rBV	589175	1066666	37.14%	5.804%
5	10.960	1277	1289	1303	rBV	236888	481882	16.78%	2.622%
6	12.370	1522	1529	1534	rVB	28473	42796	1.49%	0.233%
7	13.392	1696	1703	1710	rBV	1369421	2128837	74.13%	11.583%
8	13.592	1730	1737	1745	rBV2	38722	65455	2.28%	0.356%
9	14.091	1815	1822	1827	rBV3	20582	38626	1.34%	0.210%
10	14.250	1838	1849	1852	rBV4	15324	33554	1.17%	0.183%
11	14.661	1914	1919	1924	rBV2	41069	57849	2.01%	0.315%
12	14.767	1927	1937	1943	rVV	385713	638068	22.22%	3.472%
13	14.831	1943	1948	1954	rVB	35449	62183	2.17%	0.338%
14	15.160	2000	2004	2010	rVB2	39794	57828	2.01%	0.315%
15	15.607	2076	2080	2086	rVB	36301	50147	1.75%	0.273%
16	15.806	2109	2114	2119	rBV	48722	72491	2.52%	0.394%
17	16.100	2159	2164	2171	rVB7	14774	32383	1.13%	0.176%
18	16.247	2181	2189	2197	rBV	1198015	1873429	65.23%	10.193%
19	16.464	2222	2226	2230	rBV2	43269	70872	2.47%	0.386%
20	17.257	2356	2361	2365	rBV	40648	61898	2.16%	0.337%
21	17.322	2369	2372	2382	rVB4	29828	60613	2.11%	0.330%
22	17.510	2398	2404	2408	rBV	478690	760773	26.49%	4.139%
23	17.551	2408	2411	2417	rVV	177393	256460	8.93%	1.395%
24	17.639	2417	2426	2432	rVB	32427	67469	2.35%	0.367%
25	17.909	2469	2472	2482	rVB4	17654	35196	1.23%	0.192%
26	18.003	2483	2488	2492	rBV	35366	46580	1.62%	0.253%
27	18.174	2510	2517	2521	rVB	25764	39435	1.37%	0.215%
28	18.385	2548	2553	2558	rBV	166339	245681	8.55%	1.337%
29	18.432	2558	2561	2568	rVB2	50110	74010	2.58%	0.403%
30	18.515	2570	2575	2581	rBV6	14938	31566	1.10%	0.172%
31	18.579	2581	2586	2590	rBV5	45401	85215	2.97%	0.464%
32	18.691	2601	2605	2612	rVB	34880	51002	1.78%	0.278%
33	18.879	2632	2637	2640	rBV2	21191	30187	1.05%	0.164%
34	19.296	2703	2708	2709	rBV	35543	47329	1.65%	0.258%
35	19.431	2726	2731	2736	rBV8	16523	29498	1.03%	0.161%
36	19.554	2747	2752	2759	rVB	175275	259768	9.05%	1.413%

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37	19.654	2765	2769	2773	rBV3	48713	61305	2.13%	0.334%
38	19.801	2790	2794	2798	rBV6	17808	29983	1.04%	0.163%
39	19.889	2804	2809	2811	rBV2	62949	94608	3.29%	0.515%
40	19.919	2811	2814	2821	rVV	147069	220818	7.69%	1.201%
41	19.995	2822	2827	2831	rVB2	27852	42577	1.48%	0.232%
42	20.112	2841	2847	2853	rBV	2263791	2871937	100.00%	15.626%
43	20.412	2896	2898	2904	rVB3	47378	62660	2.18%	0.341%
44	20.712	2945	2949	2951	rBV2	21078	28736	1.00%	0.156%
45	20.917	2981	2984	2988	rVB3	32831	36048	1.26%	0.196%
46	21.182	3025	3029	3036	rVB5	17155	34220	1.19%	0.186%
47	21.340	3052	3056	3059	rBV3	23253	38722	1.35%	0.211%
48	21.428	3066	3071	3078	rBV2	228007	369706	12.87%	2.012%
49	21.681	3110	3114	3119	rVB	87715	124011	4.32%	0.675%
50	21.798	3126	3134	3139	rBV	477973	885434	30.83%	4.818%
51	22.004	3165	3169	3173	rBV6	40756	62702	2.18%	0.341%
52	22.621	3270	3274	3284	rBV7	39099	104309	3.63%	0.568%
53	23.302	3386	3390	3394	rBV6	17495	36242	1.26%	0.197%
54	25.117	3689	3699	3709	rBV2	286253	831701	28.96%	4.525%

Sum of corrected areas: 18378698

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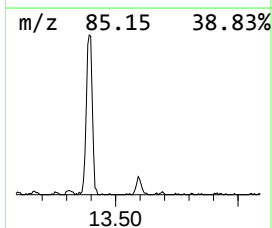
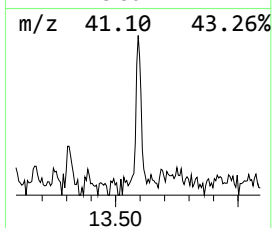
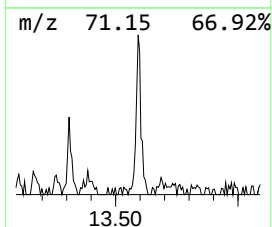
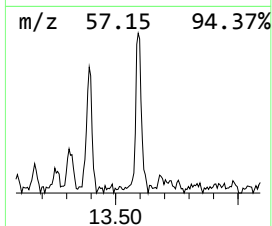
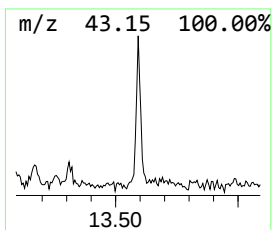
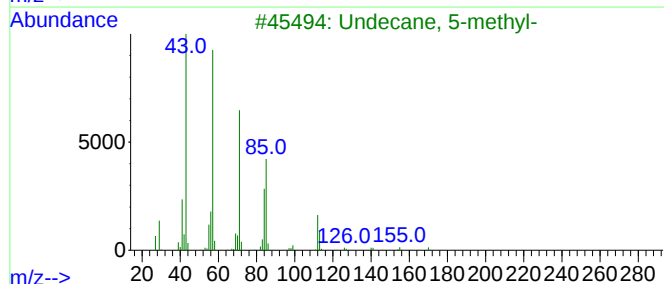
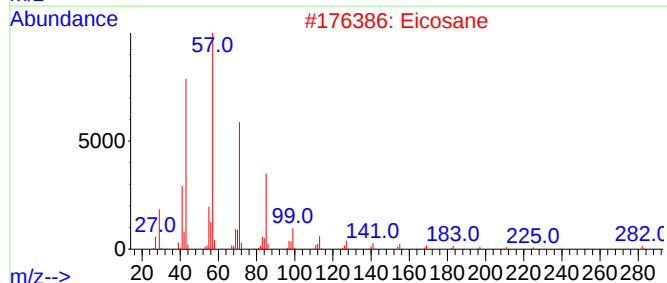
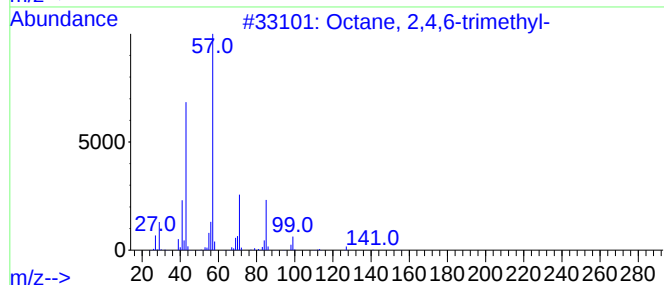
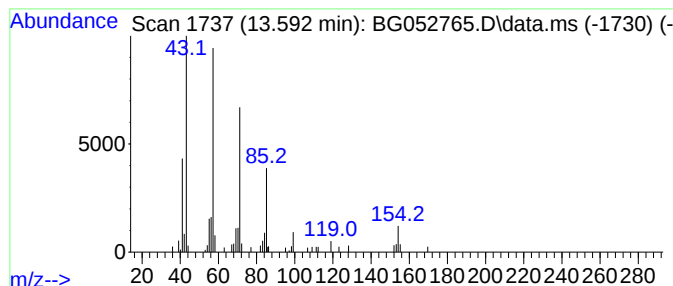
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Octane, 2,4,6-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	2.05 ng	65455	Acenaphthene-d10	14.767

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72
2			Eicosane	282	C20H42	000112-95-8	64
3			Undecane, 5-methyl-	170	C12H26	001632-70-8	64
4			Nonadecane	268	C19H40	000629-92-5	64
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



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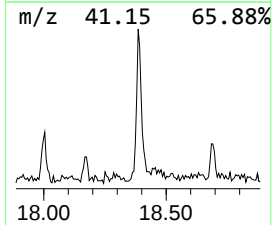
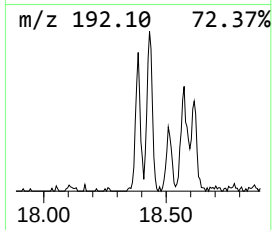
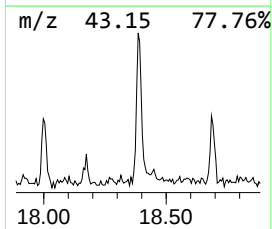
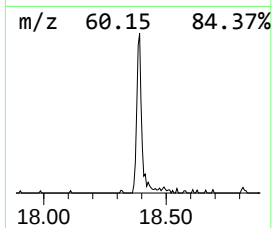
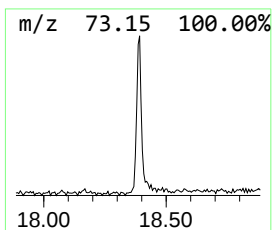
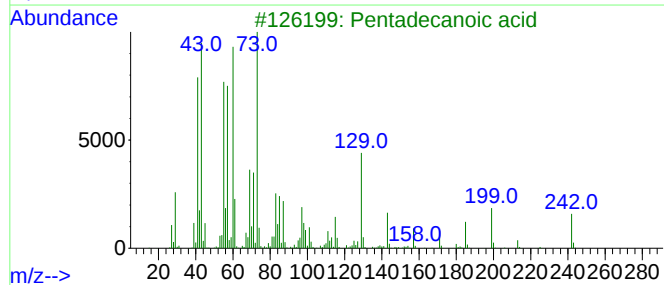
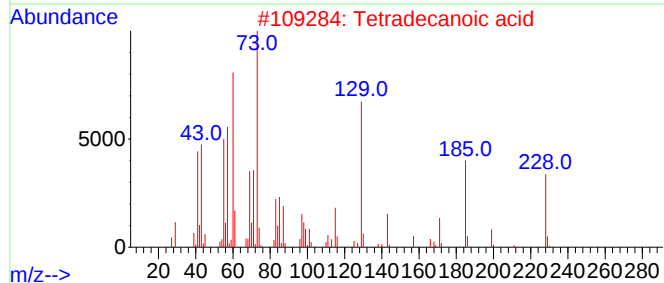
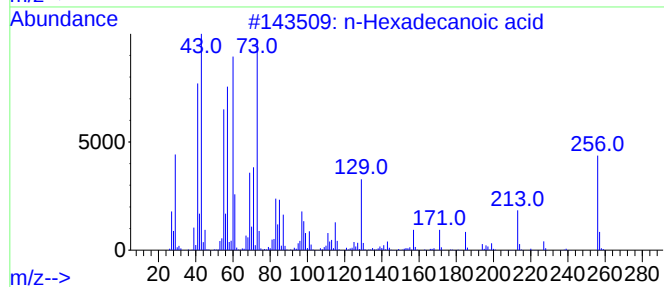
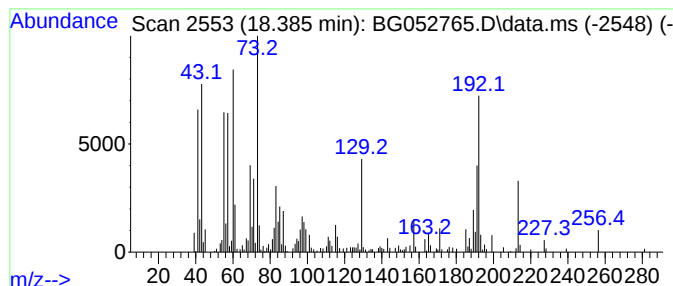
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.385	6.46 ng	245681	Phenanthrene-d10	17.510

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	55
4		Anthracene, 2-methyl-	192	C15H12	000613-12-7	47
5		Tridecanoic acid	214	C13H26O2	000638-53-9	41



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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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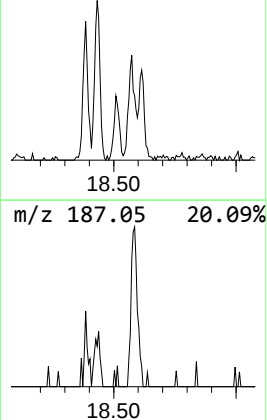
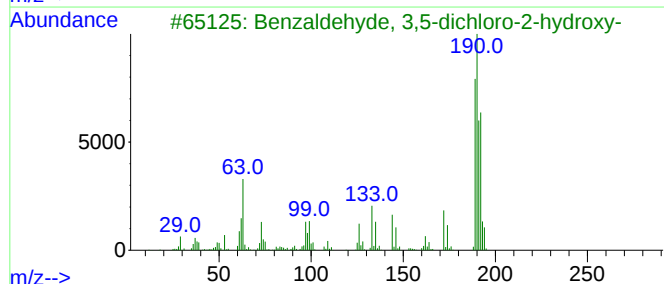
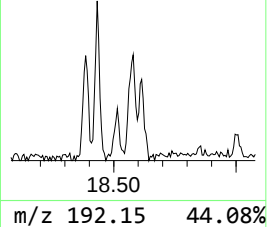
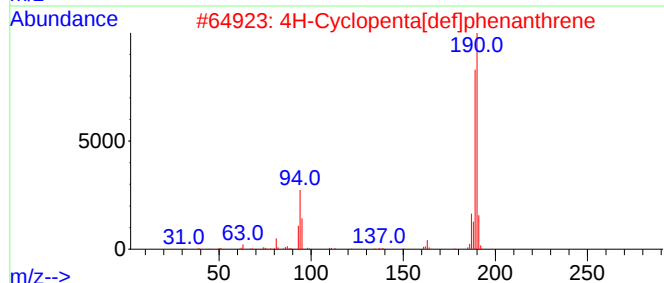
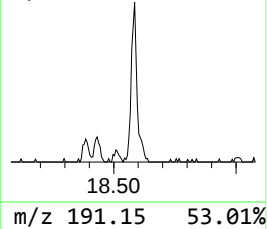
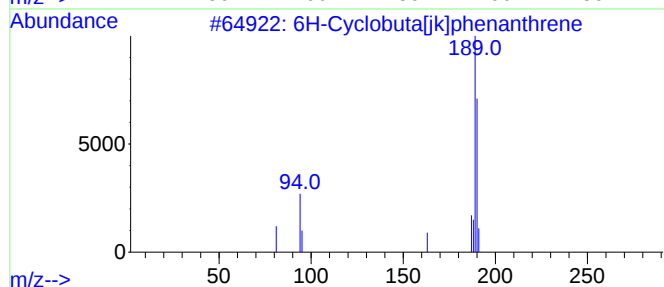
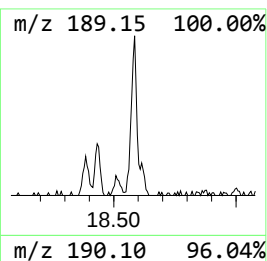
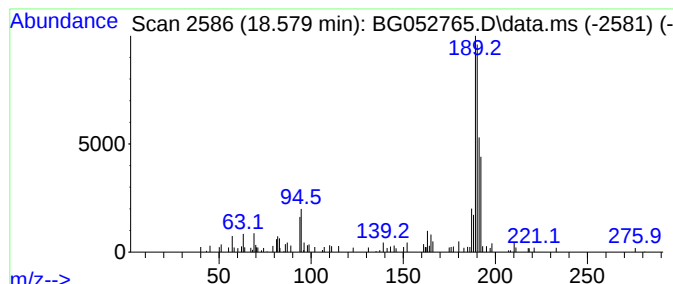
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 6H-Cyclobuta[jk]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.579	2.24 ng	85215	Phenanthrene-d10	17.510

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
2		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
3		Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
4		Benzimidazol-2(3H)-one, 5-formyl...	190	C10H10N2O2	055241-49-1	43
5		Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	38



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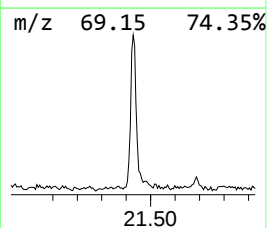
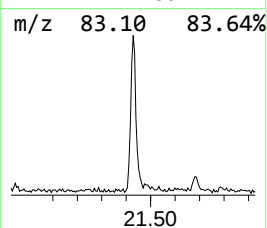
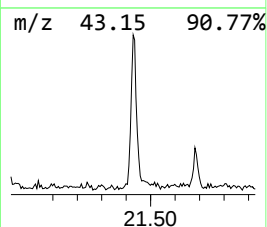
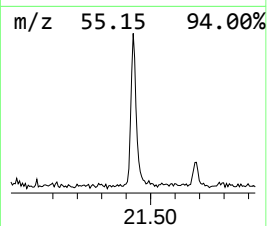
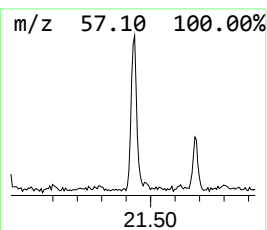
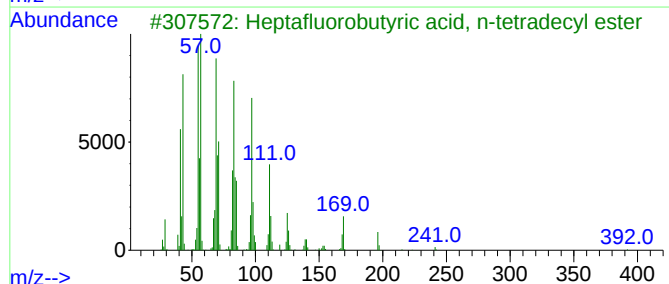
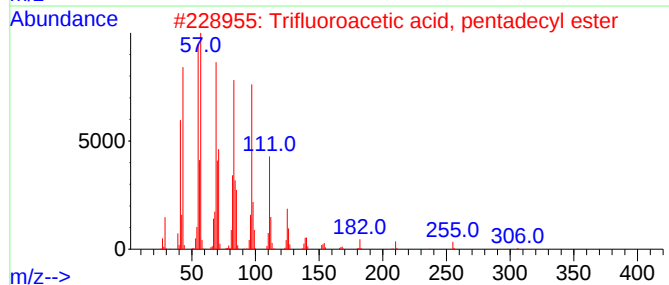
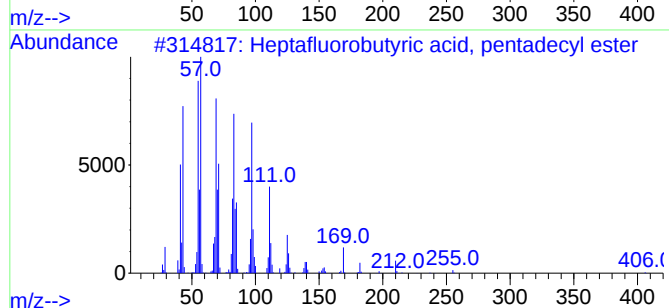
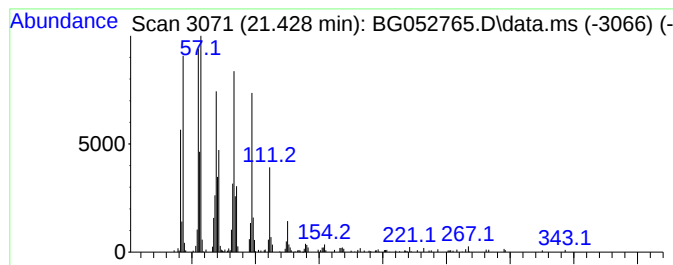
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.428	8.35 ng	369706	Chrysene-d12	21.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



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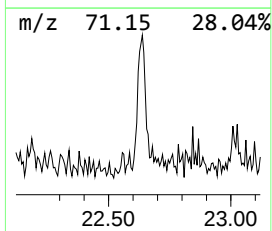
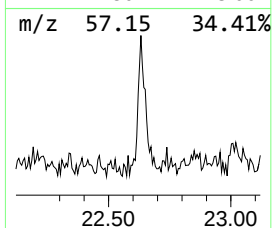
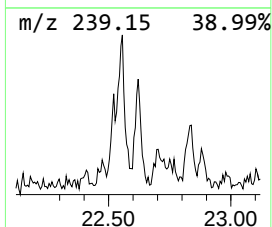
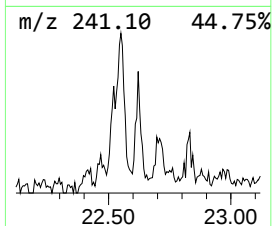
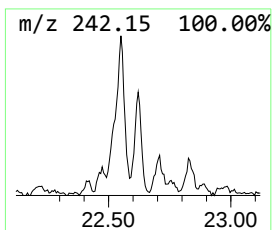
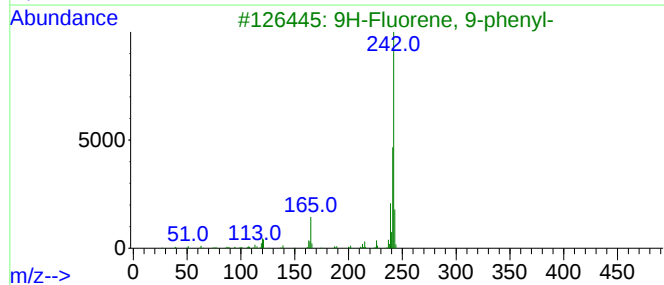
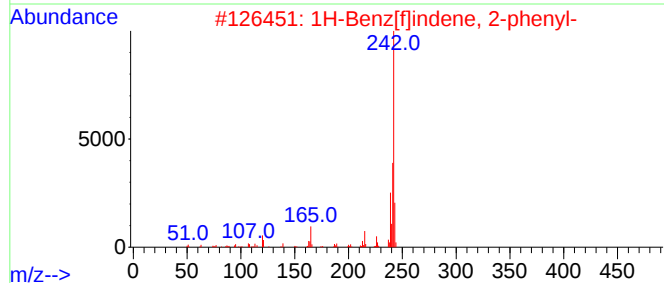
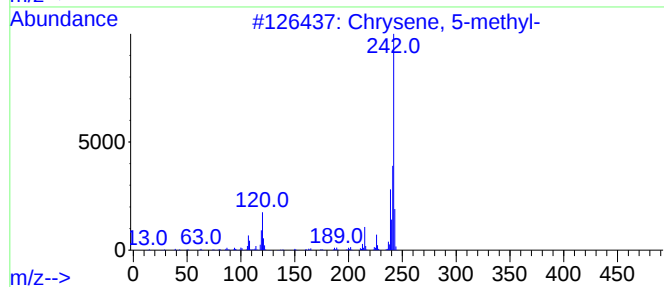
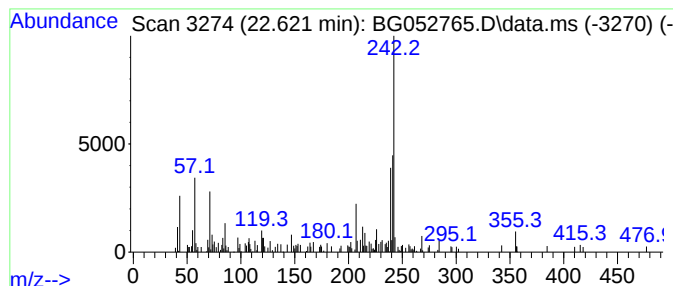
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Chrysene, 5-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.621	2.36 ng	104309	Chrysene-d12	21.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chrysene, 5-methyl-	242	C19H14	003697-24-3	55
2			1H-Benz[f]indene, 2-phenyl-	242	C19H14	1000305-22-4	46
3			9H-Fluorene, 9-phenyl-	242	C19H14	000789-24-2	46
4			Triphenylene, 1-methyl-	242	C19H14	002871-91-2	46
5			8,9-Dihydro-7H-cyclopenta[a]pyrene	242	C19H14	082979-72-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032122\
Data File : BG052765.D
Acq On : 21 Mar 2022 13:17
Operator : CG/JU
Sample : N1983-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octane, 2,4,6-t...	13.592	2.0	ng	65455	3	14.767	638068	20.0
n-Hexadecanoic ...	18.385	6.5	ng	245681	4	17.510	760773	20.0
6H-Cyclobuta[jk...	18.579	2.2	ng	85215	4	17.510	760773	20.0
Heptafluorobuty...	21.428	8.3	ng	369706	5	21.798	885434	20.0
Chrysene, 5-met...	22.621	2.4	ng	104309	5	21.798	885434	20.0