

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090722\
 Data File : BG054875.D
 Acq On : 7 Sep 2022 19:16
 Operator : CG/JU
 Sample : N4518-01 5X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SU-04-090622

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054875.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.687	402	408	418	rVB	79089	132222	11.38%	1.091%
2	7.303	676	683	691	rBV	77657	140623	12.11%	1.161%
3	8.149	820	827	835	rVB	173580	297584	25.62%	2.456%
4	9.318	1020	1026	1040	rBV	46698	95664	8.24%	0.790%
5	10.975	1301	1308	1315	rBV	243170	444321	38.25%	3.667%
6	12.620	1583	1588	1596	rVB	9998	16339	1.41%	0.135%
7	12.838	1619	1625	1632	rVB	12210	20710	1.78%	0.171%
8	13.402	1713	1721	1732	rBV	149955	238235	20.51%	1.966%
9	13.960	1806	1816	1822	rBV5	11608	27577	2.37%	0.228%
10	14.101	1834	1840	1845	rBV3	21524	38428	3.31%	0.317%
11	14.160	1845	1850	1855	rVB	10779	16634	1.43%	0.137%
12	14.336	1874	1880	1885	rBV	9890	17762	1.53%	0.147%
13	14.506	1904	1909	1917	rBV2	16427	28518	2.45%	0.235%
14	14.783	1944	1956	1962	rBV	393780	630418	54.27%	5.203%
15	14.847	1962	1967	1973	rVB	26164	41792	3.60%	0.345%
16	15.000	1984	1993	2000	rBV6	4321	12011	1.03%	0.099%
17	15.082	2000	2007	2012	rVV3	6825	13723	1.18%	0.113%
18	15.176	2014	2023	2030	rVB2	25074	46273	3.98%	0.382%
19	15.247	2030	2035	2040	rBV2	11422	18383	1.58%	0.152%
20	15.394	2053	2060	2064	rBV3	10742	21202	1.83%	0.175%
21	15.564	2080	2089	2091	rBV4	8112	17632	1.52%	0.146%
22	15.593	2091	2094	2100	rVB3	9369	12187	1.05%	0.101%
23	15.828	2127	2134	2142	rBV2	52347	90334	7.78%	0.746%
24	16.116	2175	2183	2190	rVB2	10568	24370	2.10%	0.201%
25	16.269	2197	2209	2217	rBV	104898	180257	15.52%	1.488%
26	16.492	2243	2247	2259	rVB5	9355	21440	1.85%	0.177%
27	16.827	2295	2304	2309	rBV3	20635	48115	4.14%	0.397%
28	16.880	2309	2313	2318	rVB3	12707	19412	1.67%	0.160%
29	16.974	2325	2329	2334	rVB	12553	19339	1.66%	0.160%
30	17.062	2335	2344	2347	rBV9	7943	21781	1.87%	0.180%
31	17.186	2360	2365	2369	rVB4	7869	14392	1.24%	0.119%
32	17.250	2372	2376	2383	rVV8	9519	17035	1.47%	0.141%
33	17.350	2388	2393	2399	rVB	25446	41606	3.58%	0.343%
34	17.532	2417	2424	2427	rBV	448390	705208	60.71%	5.821%
35	17.573	2427	2431	2439	rVV	305781	461616	39.74%	3.810%
36	17.662	2441	2446	2451	rVV	76676	114812	9.88%	0.948%

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37	17.720	2452	2456	2461	rVB3	13296	24069	2.07%	0.199%
38	17.938	2486	2493	2500	rBV	24520	54406	4.68%	0.449%
39	17.991	2500	2502	2507	rVV4	9178	14162	1.22%	0.117%
40	18.043	2507	2511	2515	rVV	13083	20444	1.76%	0.169%
41	18.114	2518	2523	2528	rVV	20210	37481	3.23%	0.309%
42	18.167	2528	2532	2538	rVV	129725	163078	14.04%	1.346%
43	18.249	2542	2546	2555	rVV	13278	26412	2.27%	0.218%
44	18.402	2567	2572	2577	rBV	58470	102254	8.80%	0.844%
45	18.455	2577	2581	2586	rVB	81394	119666	10.30%	0.988%
46	18.531	2590	2594	2599	rBV	28246	40928	3.52%	0.338%
47	18.602	2599	2606	2610	rBV2	109676	218732	18.83%	1.805%
48	18.801	2635	2640	2644	rBV3	8163	13873	1.19%	0.115%
49	18.843	2644	2647	2652	rBV6	9096	14552	1.25%	0.120%
50	18.895	2652	2656	2660	rVV	41989	60935	5.25%	0.503%
51	18.942	2660	2664	2675	rVB3	21507	46458	4.00%	0.383%
52	19.025	2675	2678	2682	rBV5	7965	14186	1.22%	0.117%
53	19.142	2689	2698	2702	rBV4	21360	56022	4.82%	0.462%
54	19.189	2703	2706	2710	rBV	22935	32696	2.81%	0.270%
55	19.301	2720	2725	2728	rBV2	493744	668638	57.56%	5.519%
56	19.330	2728	2730	2735	rVB2	365192	447834	38.55%	3.696%
57	19.465	2747	2753	2766	rVB2	150469	241667	20.80%	1.995%
58	19.577	2766	2772	2778	rBV	544890	800771	68.93%	6.609%
59	19.671	2785	2788	2793	rVB3	20309	29209	2.51%	0.241%
60	19.906	2824	2828	2829	rBV	64329	74971	6.45%	0.619%
61	19.941	2829	2834	2841	rVB	511825	774211	66.65%	6.390%
62	20.012	2842	2846	2850	rVB2	32684	48874	4.21%	0.403%
63	20.123	2861	2865	2870	rVB	265684	343780	29.59%	2.837%
64	20.270	2883	2890	2894	rBV2	42721	104089	8.96%	0.859%
65	20.529	2930	2934	2937	rBV	75095	99075	8.53%	0.818%
66	20.588	2941	2944	2948	rVB	60227	79134	6.81%	0.653%
67	20.723	2964	2967	2972	rBV2	68204	92876	8.00%	0.767%
68	20.776	2973	2976	2984	rVB2	57802	106147	9.14%	0.876%
69	21.827	3147	3155	3160	rBV3	474810	1161654	100.00%	9.588%
70	21.874	3160	3163	3174	rVB	204754	346993	29.87%	2.864%
71	24.130	3541	3547	3555	rBV	126919	388535	33.45%	3.207%
72	25.047	3697	3703	3719	rVB2	151148	459379	39.55%	3.792%
73	25.212	3724	3731	3740	rVB2	241970	679496	58.49%	5.608%

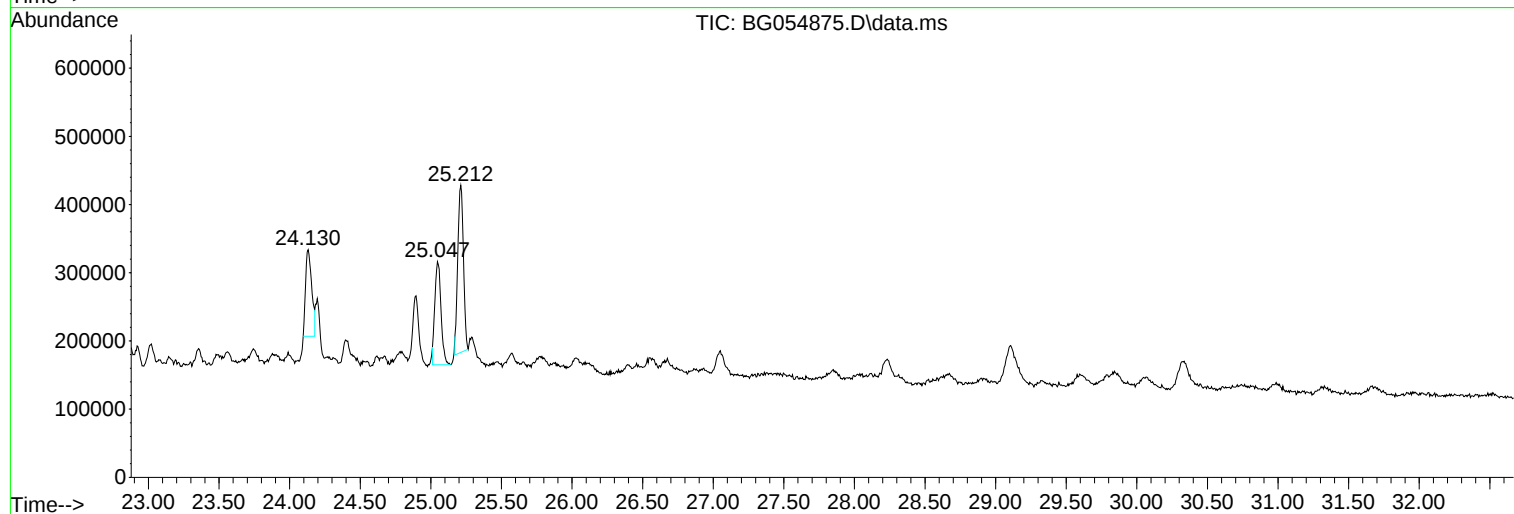
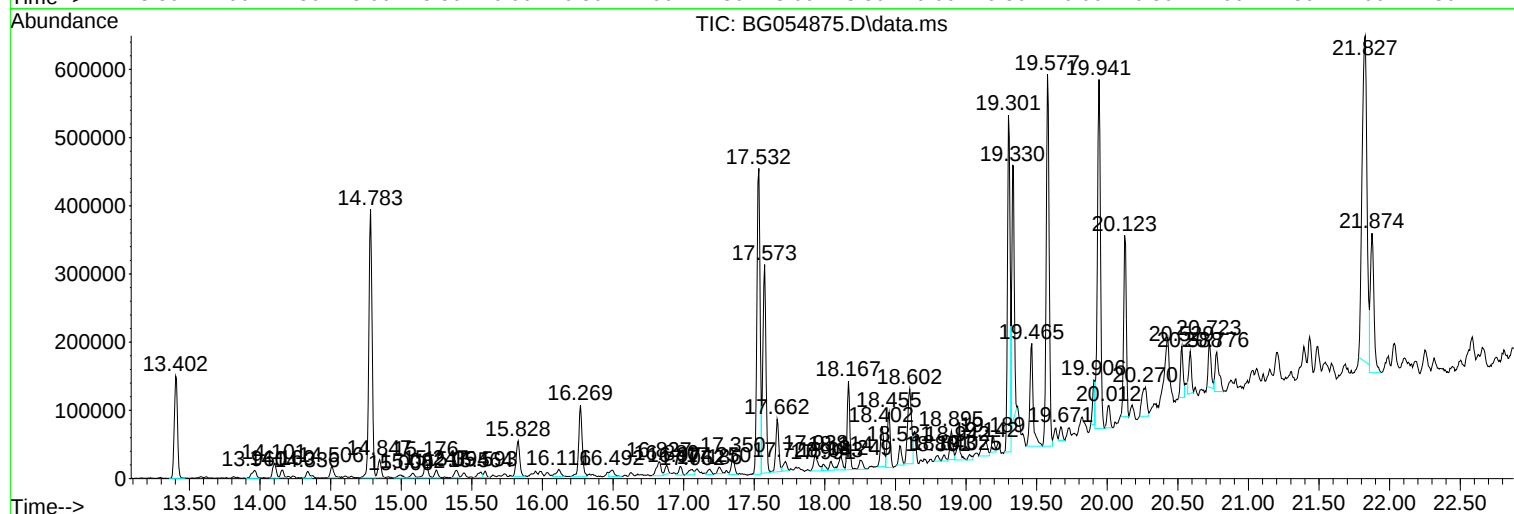
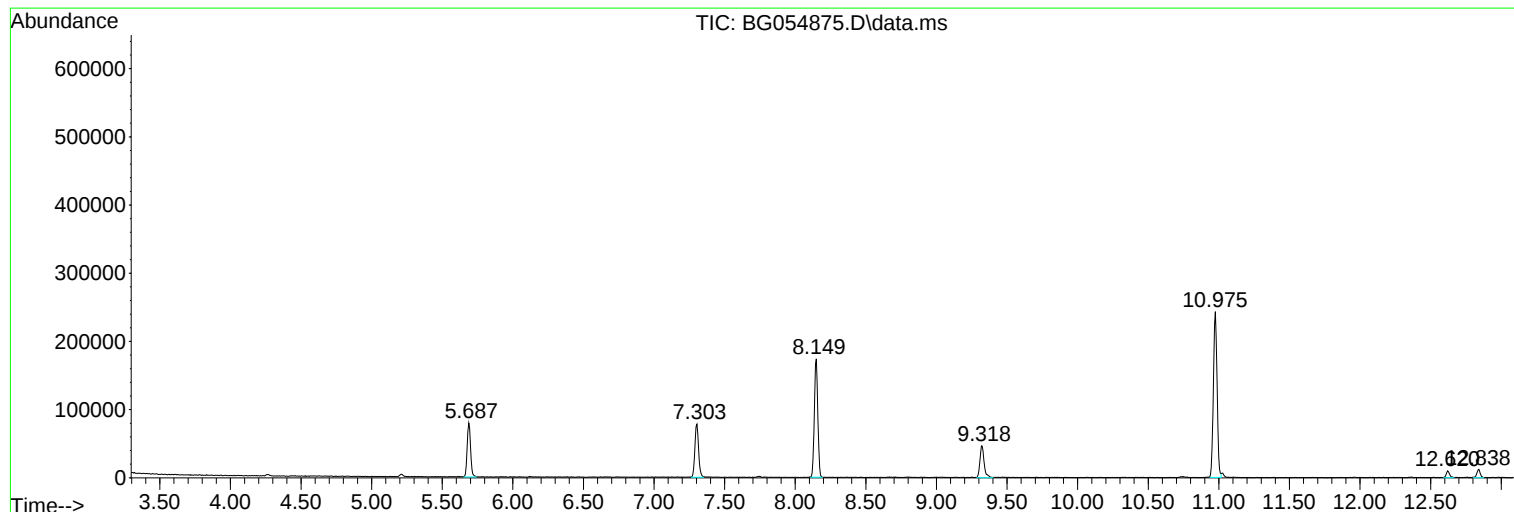
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090722\
Data File : BG054875.D
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Operator : CG/JU
Sample : N4518-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-04-090622

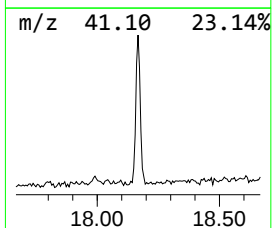
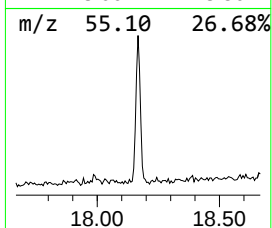
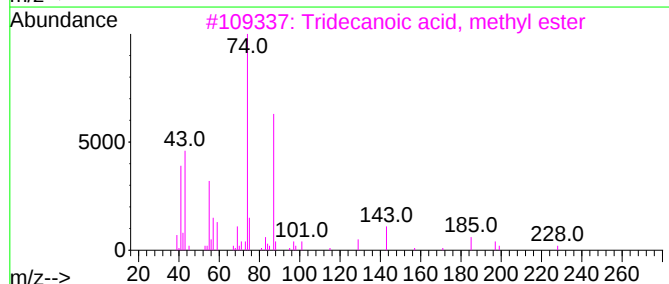
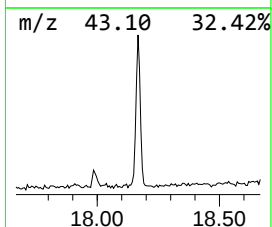
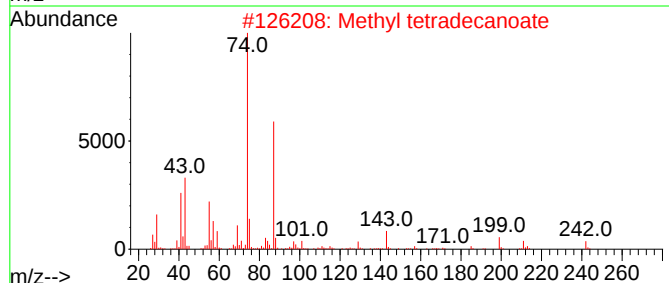
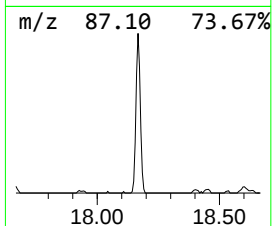
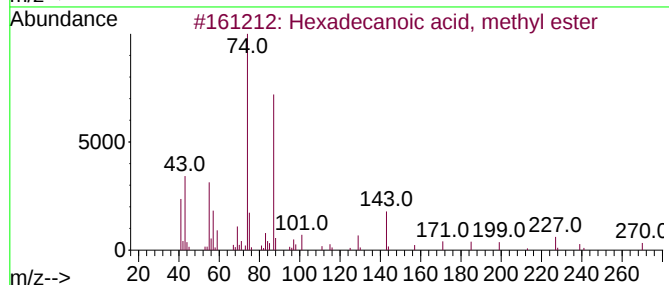
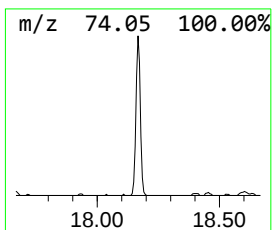
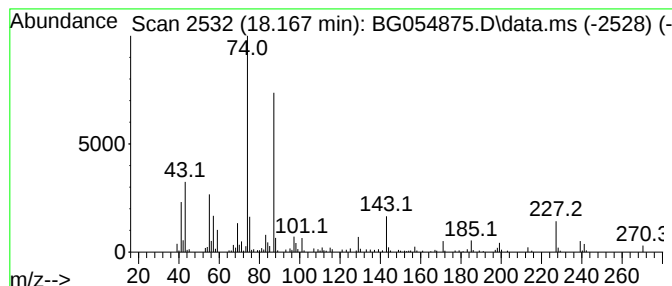
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.167	4.62 ng	163078	Phenanthrene-d10	17.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	87
5			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87



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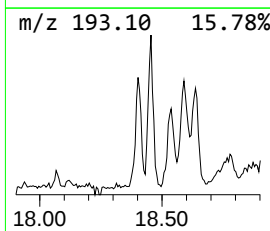
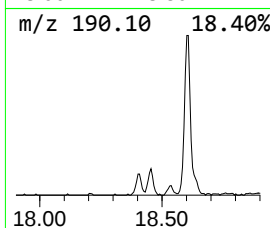
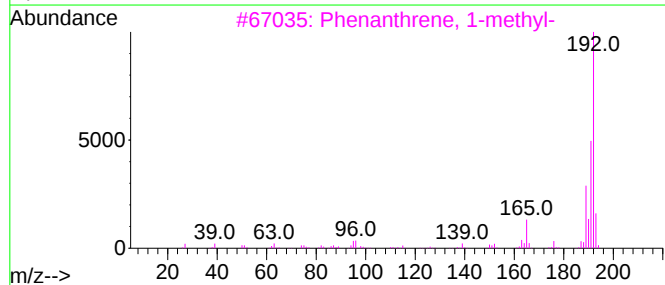
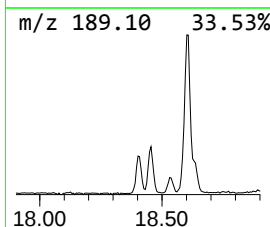
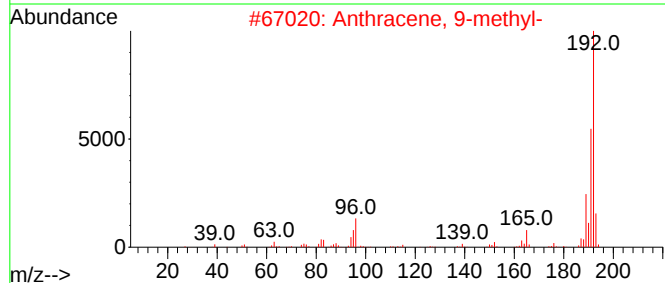
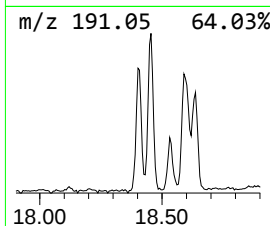
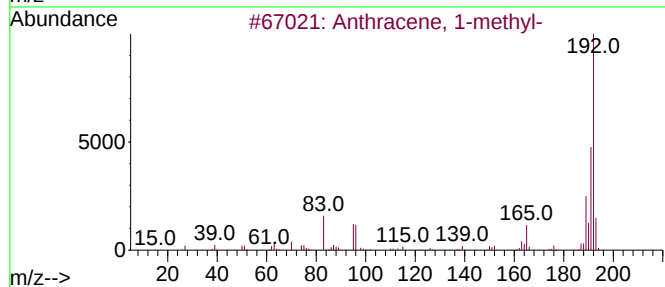
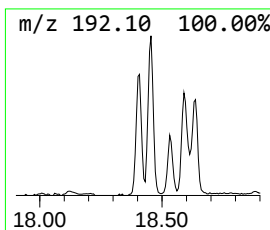
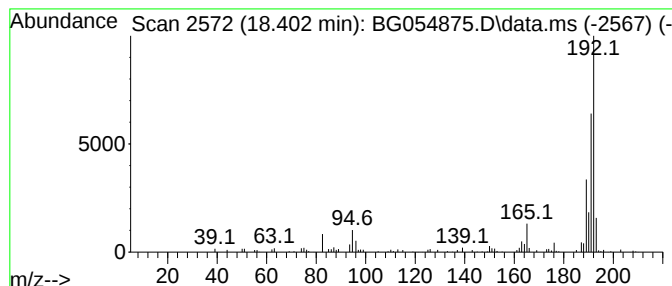
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.402	2.90 ng	102254	Phenanthrene-d10	17.532

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
2		Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
4		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90
5		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	89



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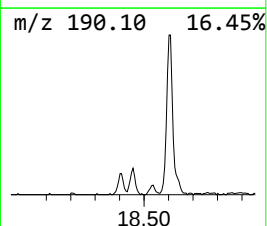
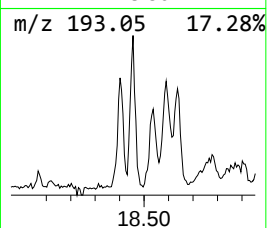
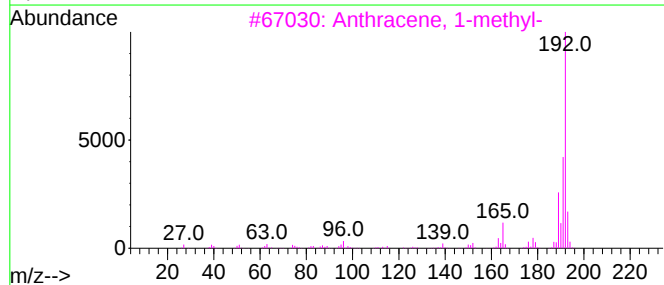
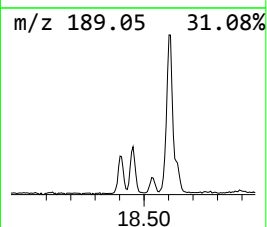
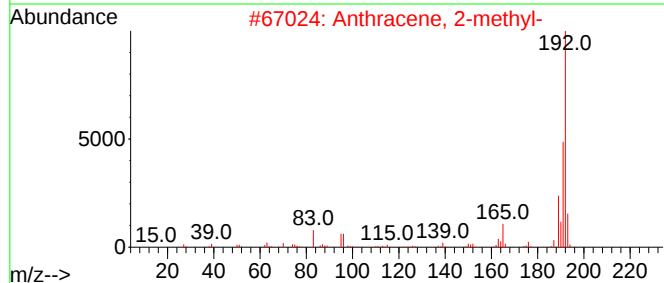
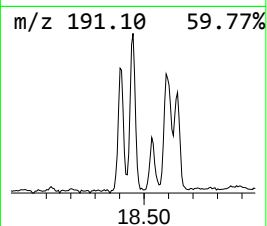
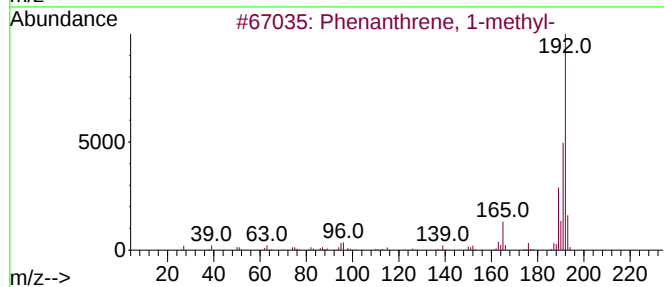
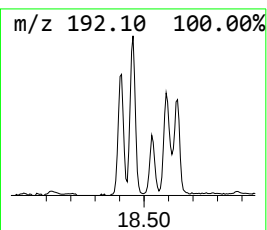
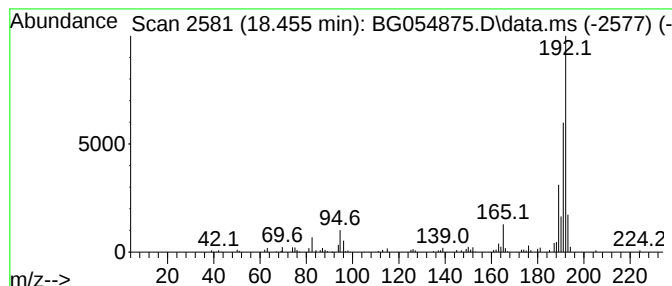
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.455	3.39 ng	119666	Phenanthrene-d10	17.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	91



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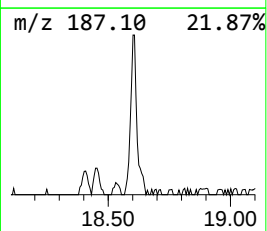
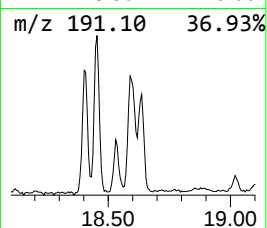
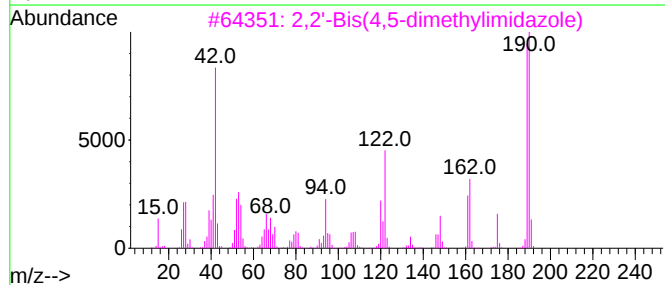
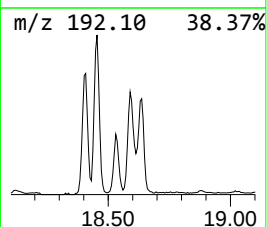
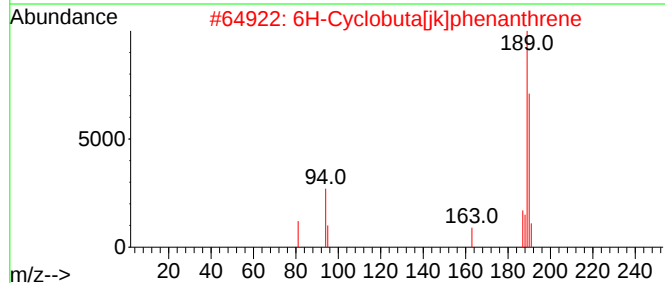
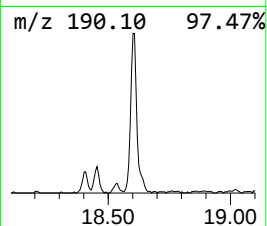
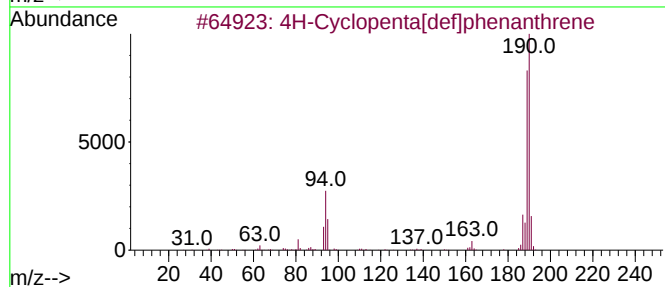
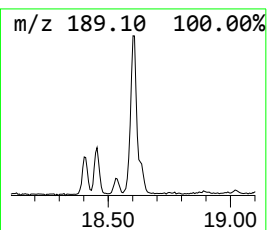
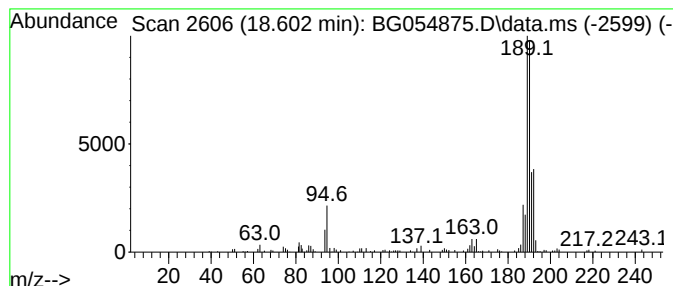
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ClientSampleId :
SU-04-090622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.602	6.20 ng	218732	Phenanthrene-d10	17.532	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	86
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	1-Aminocyclopentanecarboxylic ac...	361	C18H32ClN04	1000329-17-0	35
5	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090722\
Data File : BG054875.D
Acq On : 7 Sep 2022 19:16
Operator : CG/JU
Sample : N4518-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

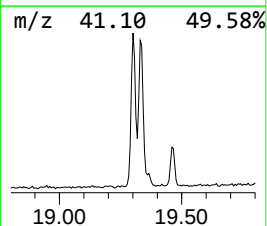
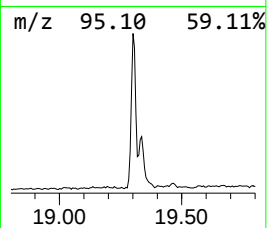
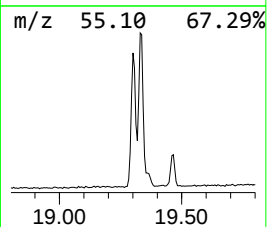
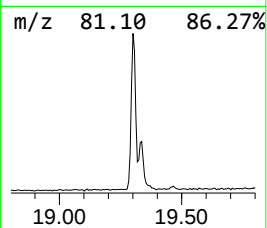
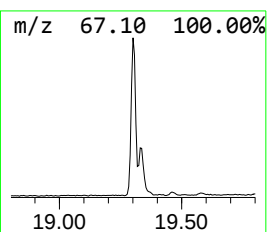
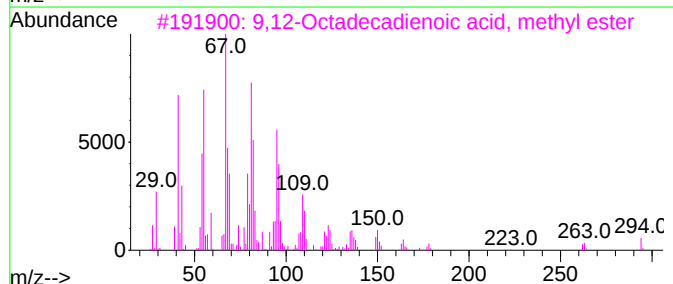
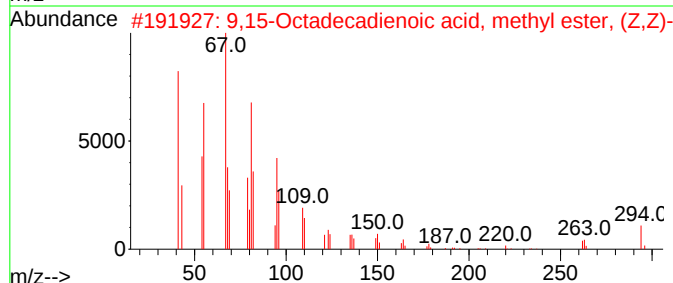
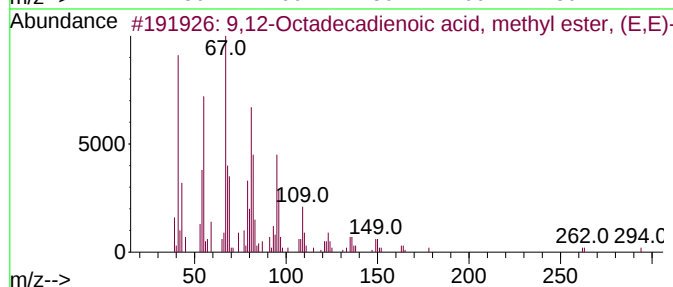
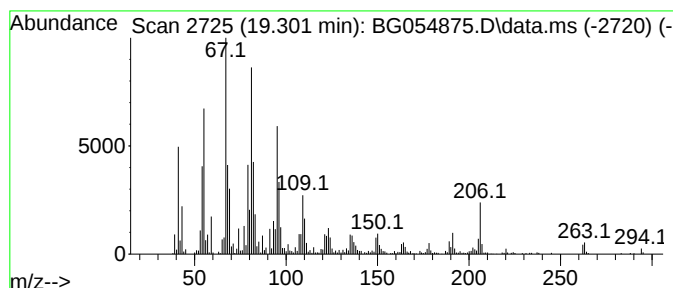
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ClientSampleId :
SU-04-090622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.301	18.96 ng	668638	Phenanthrene-d10	17.532	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090722\
Data File : BG054875.D
Acq On : 7 Sep 2022 19:16
Operator : CG/JU
Sample : N4518-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

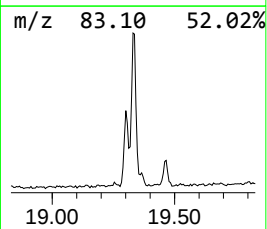
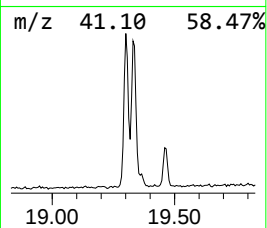
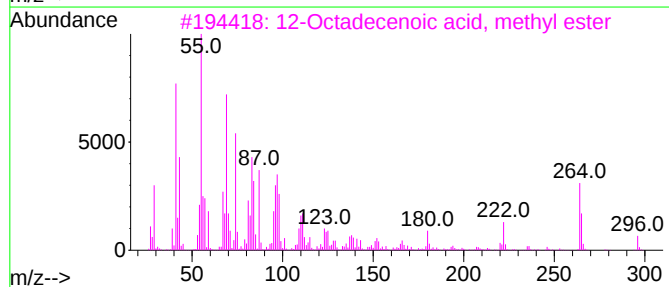
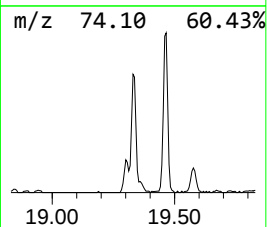
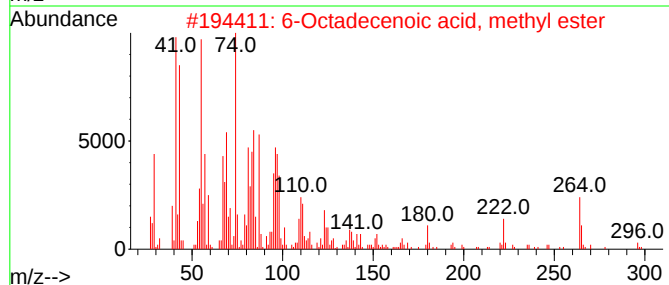
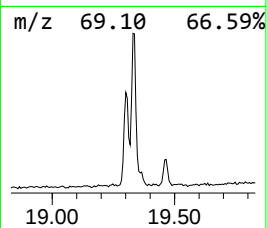
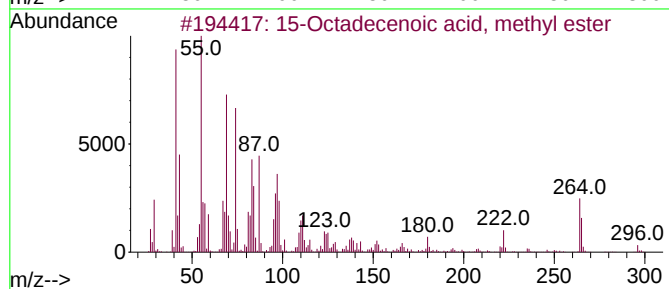
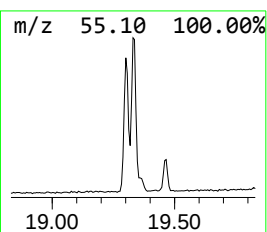
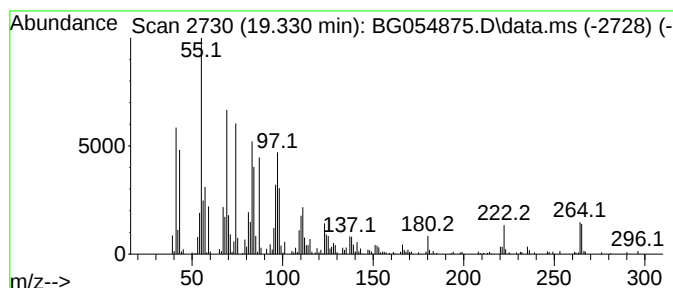
Instrument :
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ClientSampleId :
SU-04-090622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 15-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.330	12.70 ng	447834	Phenanthrene-d10	17.532	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	95
2	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	94
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090722\
Data File : BG054875.D
Acq On : 7 Sep 2022 19:16
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Sample : N4518-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

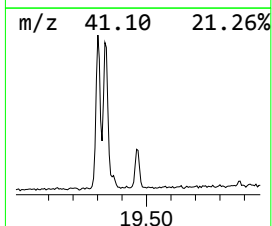
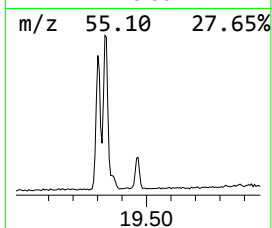
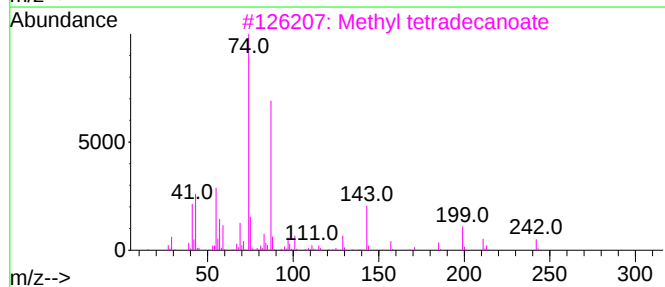
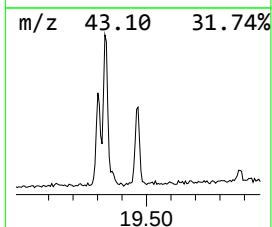
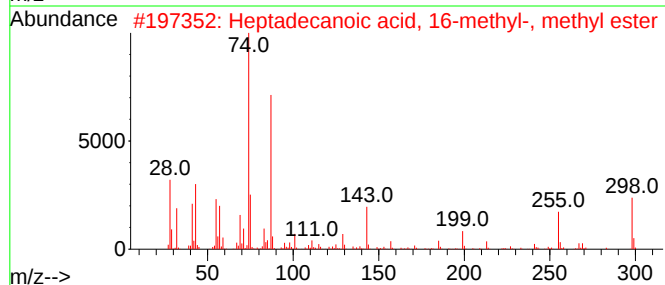
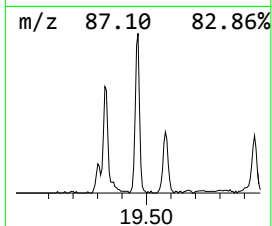
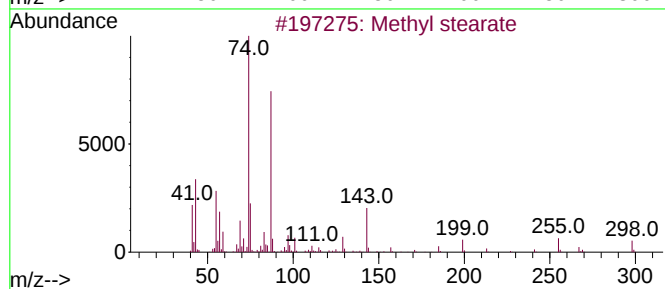
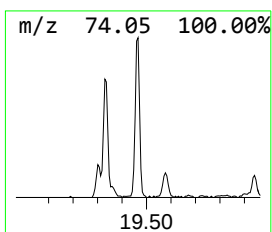
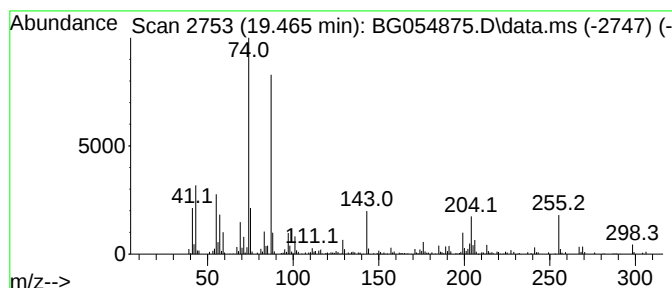
Instrument :
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ClientSampleId :
SU-04-090622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.465	6.85 ng	241667	Phenanthrene-d10		17.532	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Methyl stearate		298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...		298	C19H38O2	005129-61-3	89
3	Methyl tetradecanoate		242	C15H30O2	000124-10-7	83
4	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	80
5	Methyl 8-methyl-nonanoate		186	C11H22O2	1000452-00-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090722\
Data File : BG054875.D
Acq On : 7 Sep 2022 19:16
Operator : CG/JU
Sample : N4518-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-04-090622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
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Anthracene, 1-m...	18.402	2.9	ng	102254	4	17.532	705208	20.0
Phenanthrene, 1...	18.455	3.4	ng	119666	4	17.532	705208	20.0
4H-Cyclopenta[d...	18.602	6.2	ng	218732	4	17.532	705208	20.0
9,12-Octadecadi...	19.301	19.0	ng	668638	4	17.532	705208	20.0
15-Octadecenoic...	19.330	12.7	ng	447834	4	17.532	705208	20.0
Methyl stearate	19.465	6.8	ng	241667	4	17.532	705208	20.0