

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
 Data File : BG064097.D
 Acq On : 11 Mar 2025 15:56
 Operator : RC/JU
 Sample : Q1534-13
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OR-363-COMP-18

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-BG030525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG064097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.992	319	324	329	rBV2	15715	24458	1.08%	0.144%
2	5.456	394	403	411	rBV	780751	1216930	53.54%	7.153%
3	7.031	662	671	688	rBV	831206	1377964	60.63%	8.100%
4	7.865	806	813	819	rBV	162005	267297	11.76%	1.571%
5	9.017	1000	1009	1017	rBV	474863	841722	37.03%	4.948%
6	9.575	1096	1104	1112	rBV3	29269	46421	2.04%	0.273%
7	10.650	1280	1287	1294	rBV	218261	375500	16.52%	2.207%
8	13.112	1699	1706	1714	rBV	1081720	1616443	71.12%	9.502%
9	14.487	1930	1940	1946	rBV	324366	506742	22.30%	2.979%
10	15.844	2164	2171	2178	rVB	222833	300069	13.20%	1.764%
11	15.973	2186	2193	2201	rBV	949941	1419790	62.47%	8.346%
12	17.225	2399	2406	2410	rBV	405783	609937	26.84%	3.585%
13	17.266	2410	2413	2419	rVB	94602	138375	6.09%	0.813%
14	18.083	2545	2552	2553	rBV4	19346	32204	1.42%	0.189%
15	18.135	2553	2561	2574	rVB2	272473	468434	20.61%	2.753%
16	18.288	2583	2587	2592	rBV4	21582	36948	1.63%	0.217%
17	18.500	2618	2623	2631	rBV6	55474	95698	4.21%	0.563%
18	18.635	2643	2646	2652	rVB5	24247	32616	1.44%	0.192%
19	19.128	2725	2730	2732	rBV5	15405	24134	1.06%	0.142%
20	19.275	2749	2755	2764	rBV	315957	470308	20.69%	2.764%
21	19.404	2773	2777	2784	rBV4	54857	99679	4.39%	0.586%
22	19.640	2805	2817	2825	rBV	258358	486071	21.39%	2.857%
23	19.757	2833	2837	2843	rVB3	28219	36536	1.61%	0.215%
24	19.845	2843	2852	2861	rBV	1698644	2272879	100.00%	13.360%
25	19.951	2865	2870	2878	rVV6	40375	75228	3.31%	0.442%
26	20.133	2897	2901	2906	rVB2	40496	57483	2.53%	0.338%
27	20.233	2914	2918	2922	rBV3	16535	25450	1.12%	0.150%
28	20.286	2923	2927	2931	rVV4	21427	30997	1.36%	0.182%
29	20.480	2956	2960	2964	rVV6	14083	24255	1.07%	0.143%
30	20.544	2967	2971	2977	rVB5	22880	42224	1.86%	0.248%
31	20.621	2981	2984	2988	rVB	28045	28825	1.27%	0.169%
32	20.879	3024	3028	3035	rVB2	34874	61234	2.69%	0.360%
33	21.055	3050	3058	3062	rBV3	36898	82065	3.61%	0.482%
34	21.097	3062	3065	3068	rVV4	27559	37148	1.63%	0.218%
35	21.138	3068	3072	3078	rVV2	185557	293308	12.90%	1.724%
36	21.197	3078	3082	3086	rVB2	37248	62277	2.74%	0.366%

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37	21.379	3108	3113	3116	rBV	31599	44996	1.98%	0.264%
38	21.455	3118	3126	3131	rVV2	472814	975562	42.92%	5.734%
39	21.502	3131	3134	3141	rVB	162013	241744	10.64%	1.421%
40	21.649	3155	3159	3162	rBV3	17131	29553	1.30%	0.174%
41	21.843	3186	3192	3198	rBV6	20536	46735	2.06%	0.275%
42	22.148	3242	3244	3250	rVB3	22246	30566	1.34%	0.180%
43	22.219	3252	3256	3259	rVV5	20973	34392	1.51%	0.202%
44	22.260	3259	3263	3267	rVB4	23202	38530	1.70%	0.226%
45	22.865	3362	3366	3372	rBV5	24866	40599	1.79%	0.239%
46	23.077	3398	3402	3410	rVB2	36096	65565	2.88%	0.385%
47	23.523	3469	3478	3485	rBV	122292	396766	17.46%	2.332%
48	23.664	3496	3502	3506	rBV4	30615	63260	2.78%	0.372%
49	24.187	3586	3591	3603	rVB2	63135	168067	7.39%	0.988%
50	24.328	3608	3615	3629	rVB2	83131	230815	10.16%	1.357%
51	24.475	3629	3640	3648	rBV3	257741	727948	32.03%	4.279%
52	24.546	3648	3652	3658	rVB3	33540	62284	2.74%	0.366%
53	25.603	3823	3832	3839	rBV3	38580	107854	4.75%	0.634%
54	25.703	3843	3849	3860	rVB9	27340	89530	3.94%	0.526%

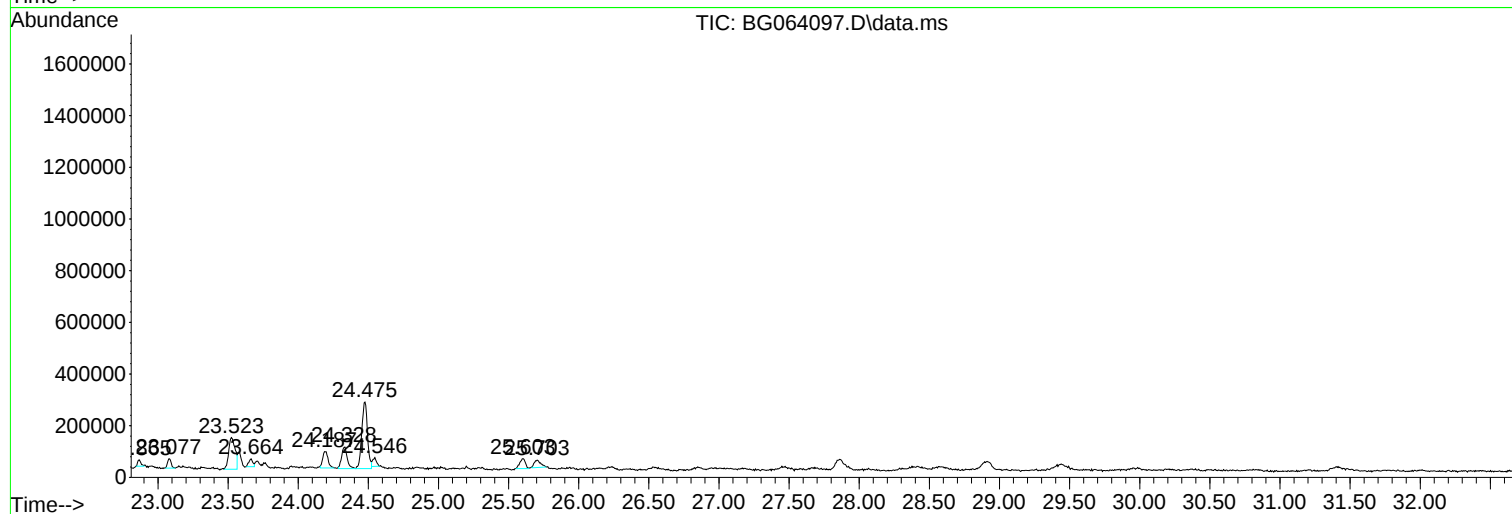
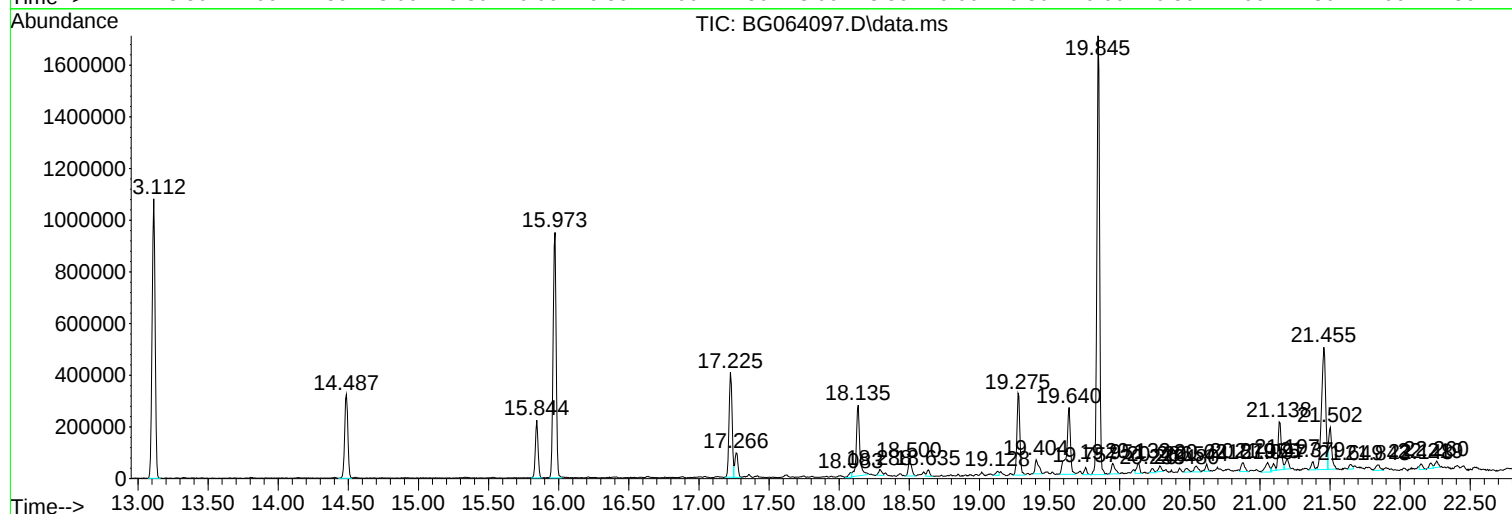
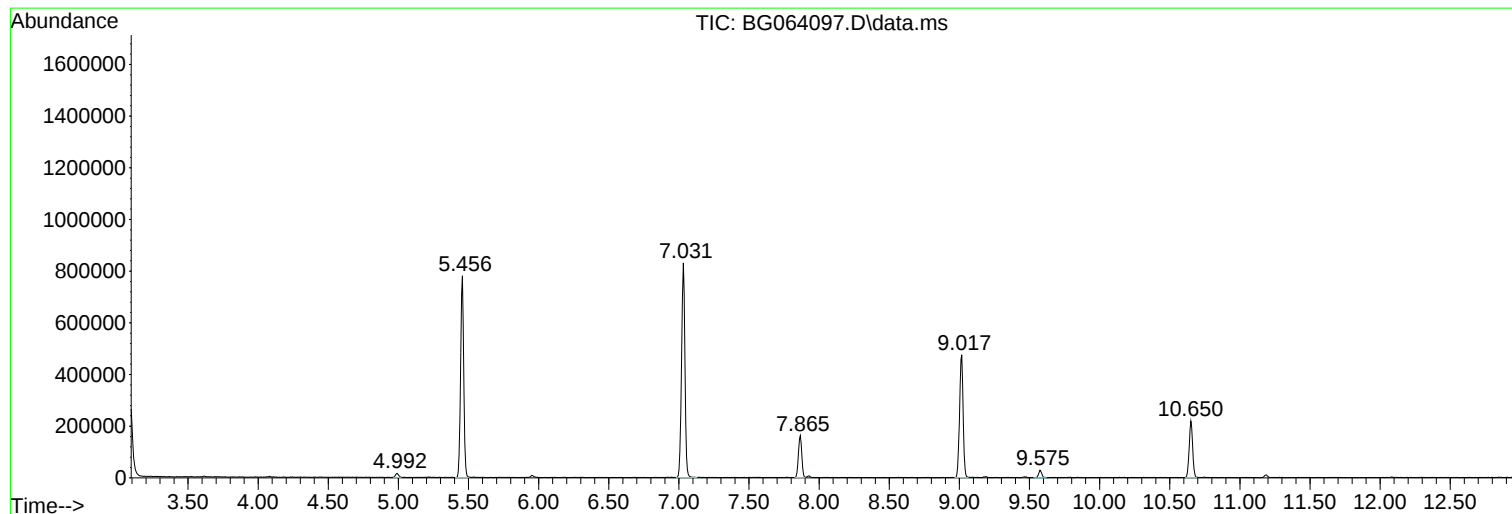
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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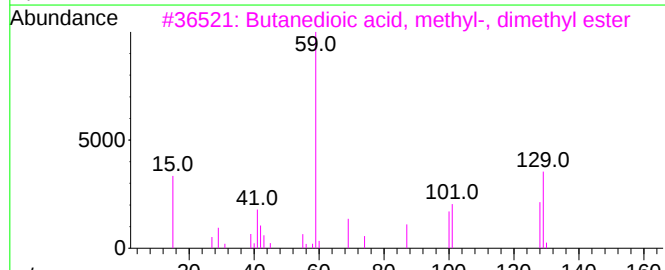
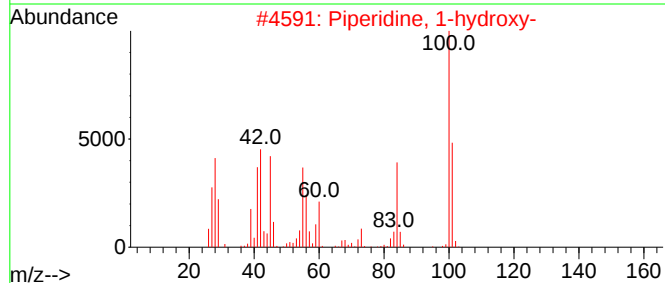
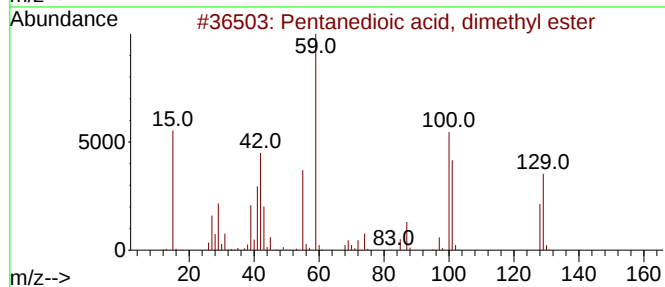
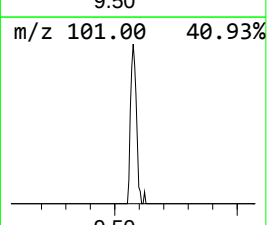
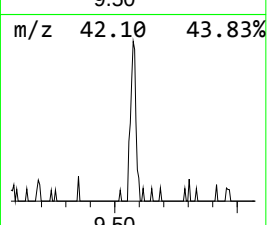
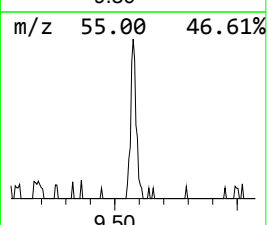
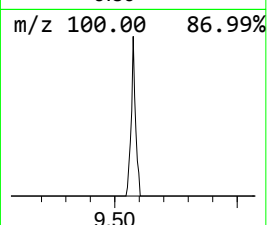
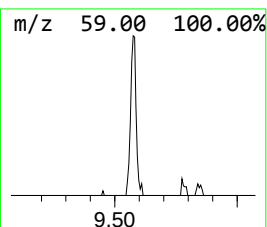
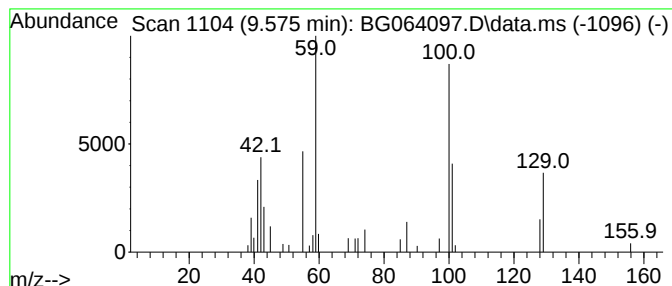
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.575	2.47 ng	46421	Naphthalene-d8	10.650

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	64
2			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	37
3			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	23
4			1,3-Bis(dimethyl-n-pentylsilyl)b...	312	C18H40Si2	136935-59-6	22
5			Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	17



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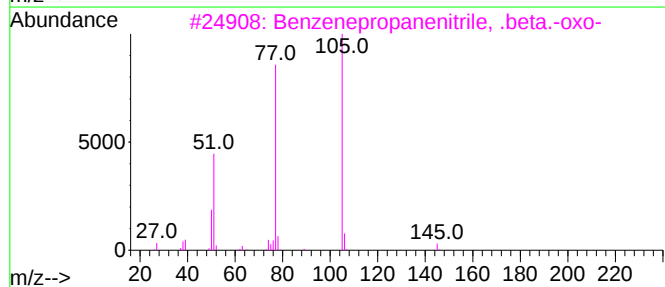
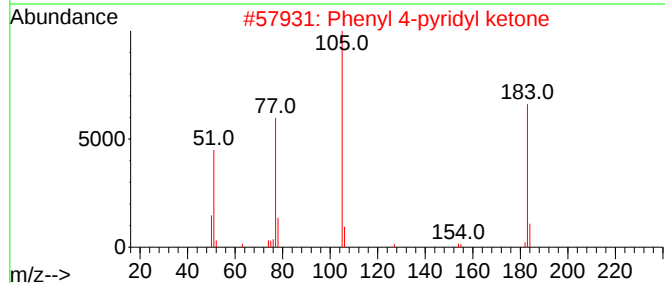
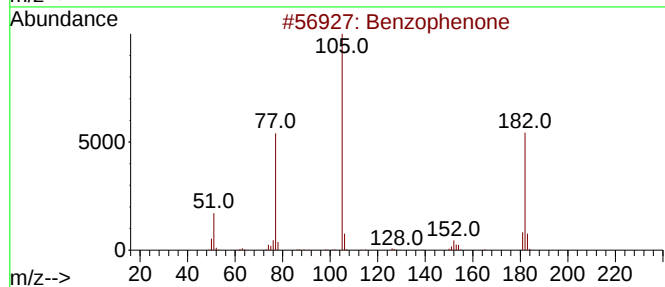
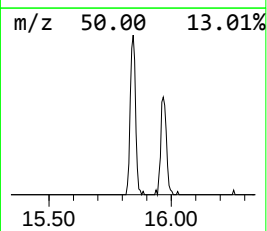
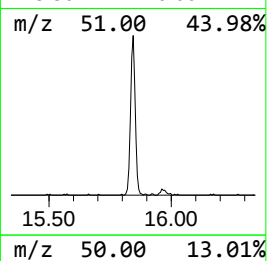
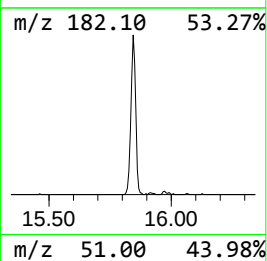
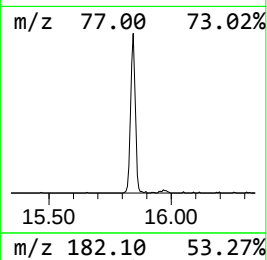
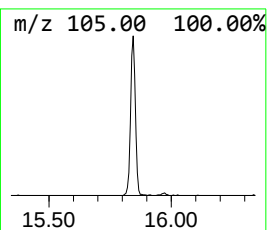
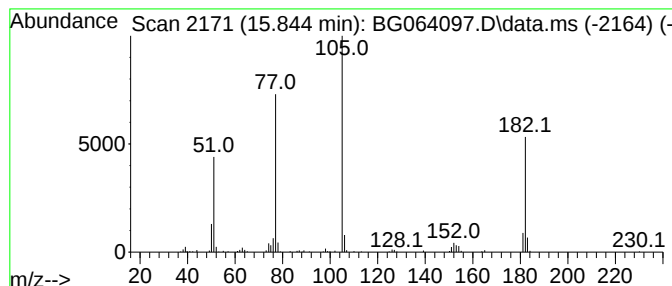
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.844	11.84 ng	300069	Acenaphthene-d10	14.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	52
4			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	50
5			Acetic acid, 2-benzoylthio-, 2-o...	314	C17H14O4S	1000260-20-1	50



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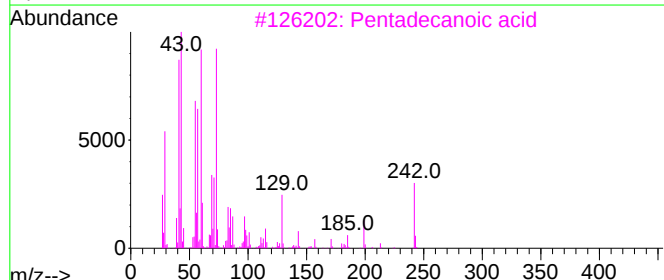
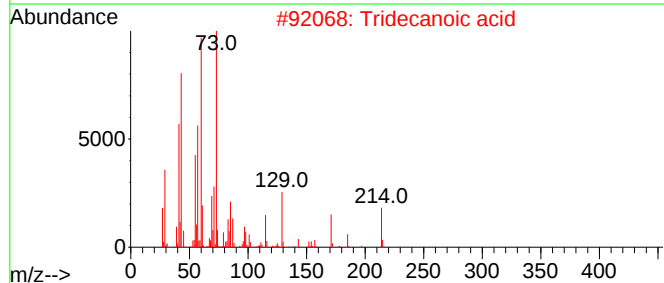
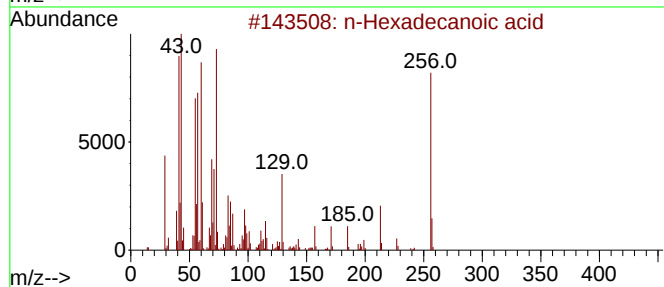
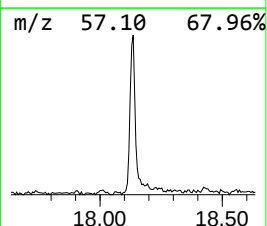
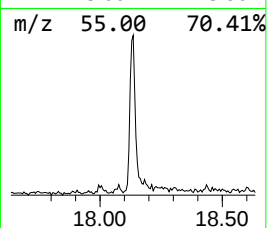
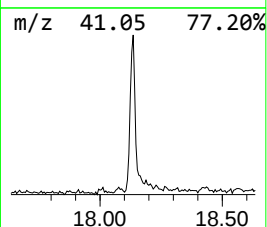
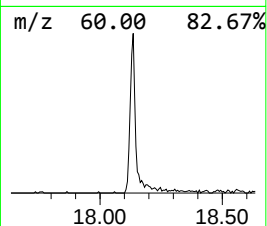
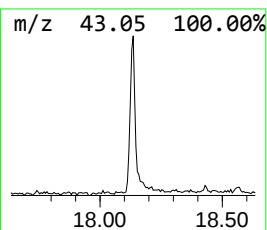
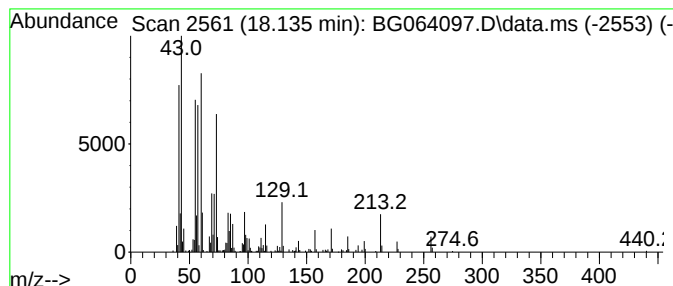
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.135	15.36 ng	468434	Phenanthrene-d10	17.225

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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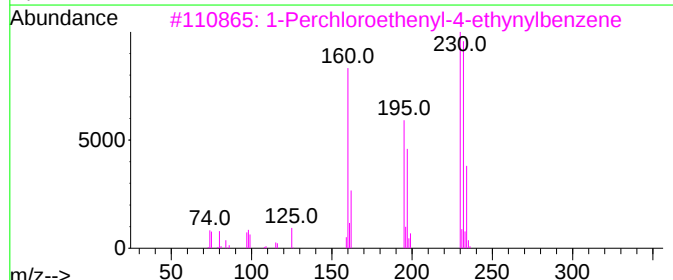
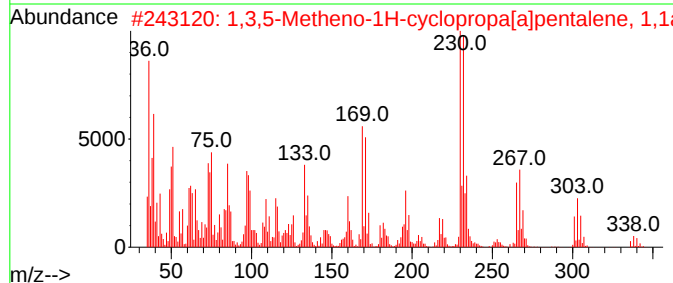
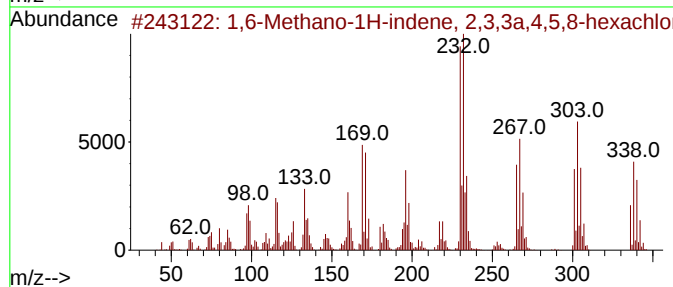
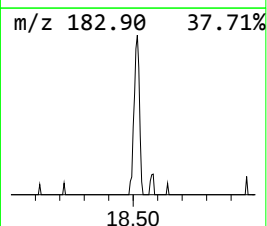
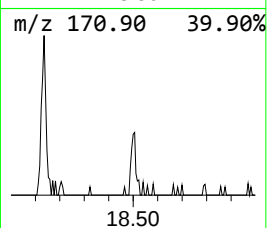
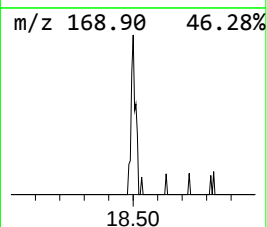
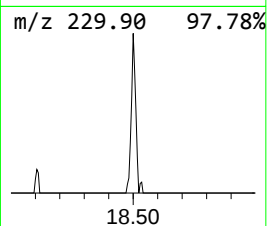
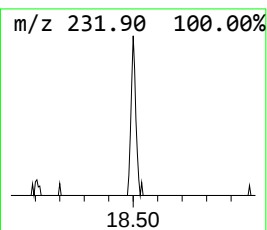
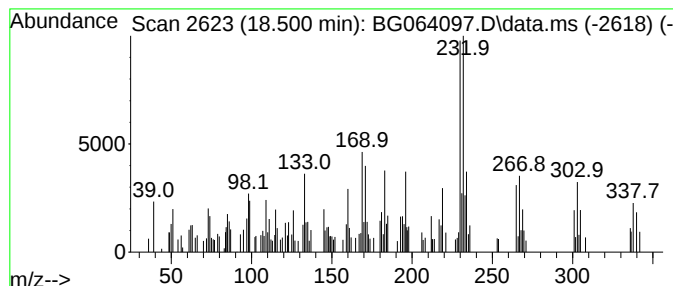
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,6-Methano-1H-indene, 2,3,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.500	3.14 ng	95698	Phenanthrene-d10	17.225

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Methano-1H-indene, 2,3,3a,4,...	336	C10H6Cl6	056641-38-4	96		
2	1,3,5-Metheno-1H-cyclopropa[a]pe...	336	C10H6Cl6	069743-71-1	87		
3	1-Perchloroethenyl-4-ethynylbenzene	230	C10H5Cl3	1000283-76-9	55		
4	Naphthalene, 1,3,7-trichloro-	230	C10H5Cl3	055720-37-1	46		
5	6-Bromo-4-chloro-1H-indazole	230	C7H4BrClN2	885518-99-0	46		



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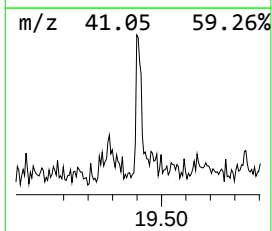
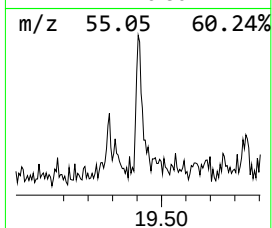
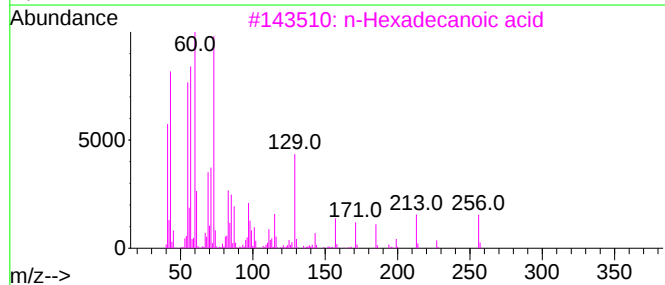
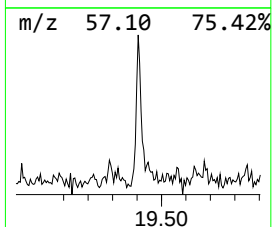
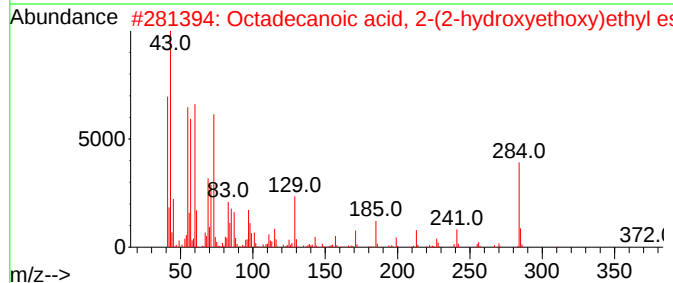
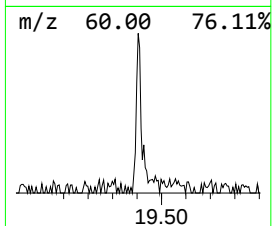
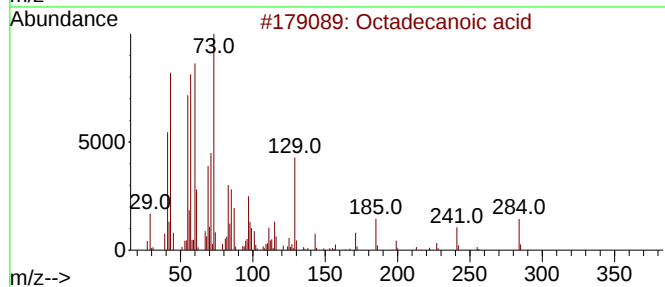
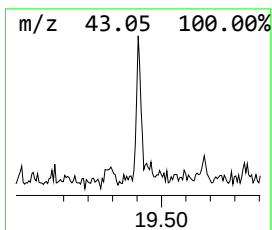
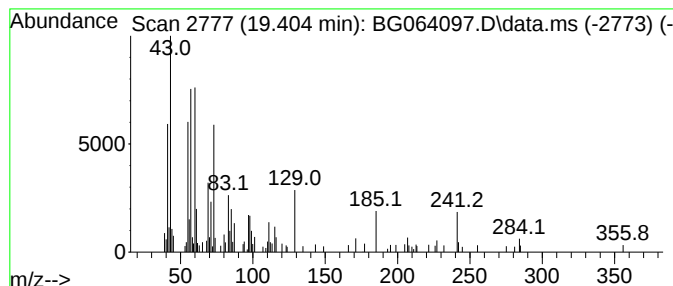
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	2.04 ng	99679	Chrysene-d12	21.455

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	83
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
Data File : BG064097.D
Acq On : 11 Mar 2025 15:56
Operator : RC/JU
Sample : Q1534-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-18

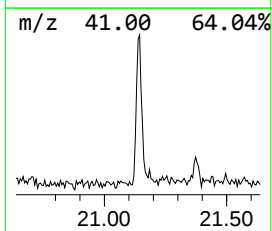
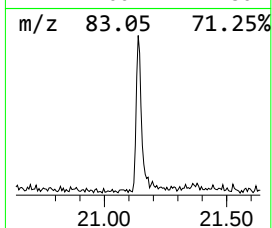
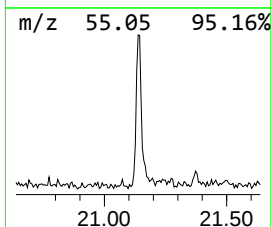
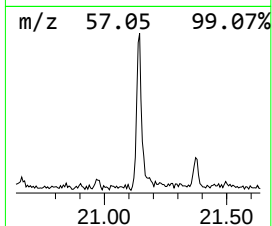
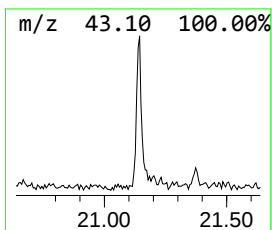
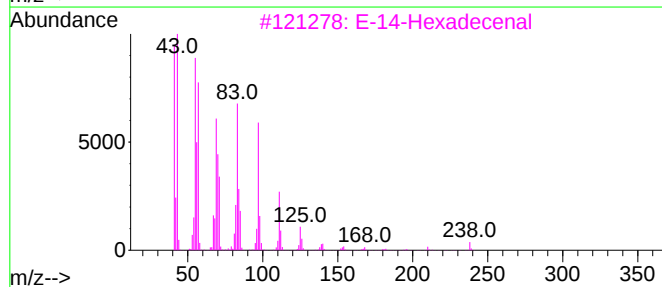
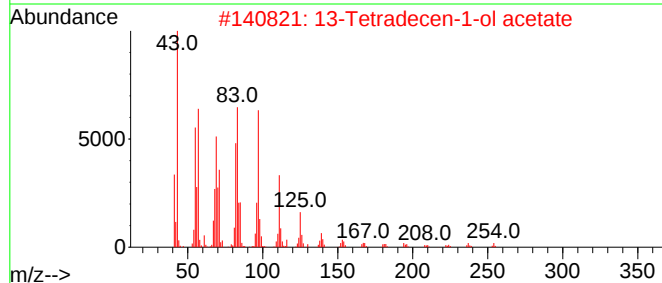
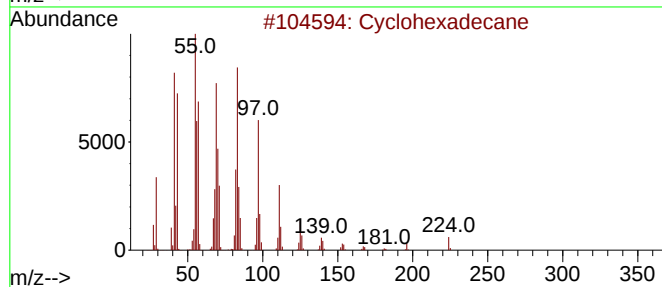
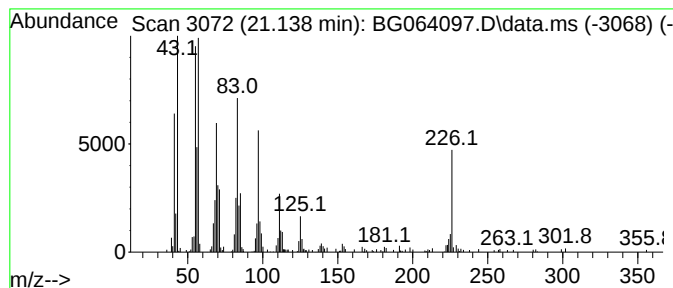
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.138	6.01 ng	293308	Chrysene-d12	21.455

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	99
2			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	83
3			E-14-Hexadecenal	238	C16H30O	330207-53-9	83
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	81
5			Cetene	224	C16H32	000629-73-2	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
Data File : BG064097.D
Acq On : 11 Mar 2025 15:56
Operator : RC/JU
Sample : Q1534-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-18

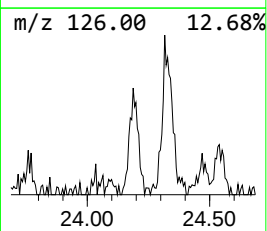
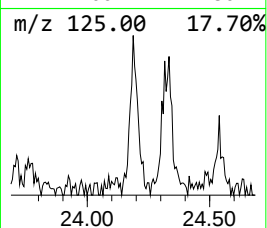
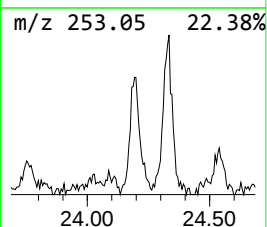
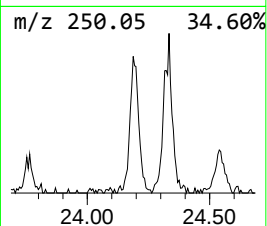
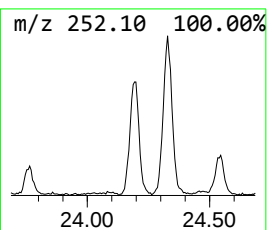
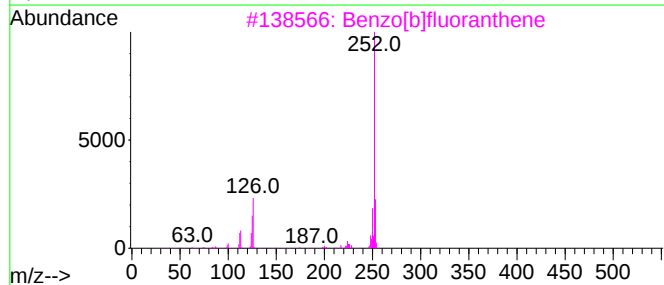
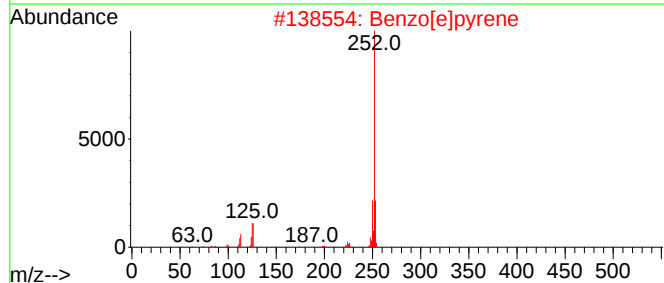
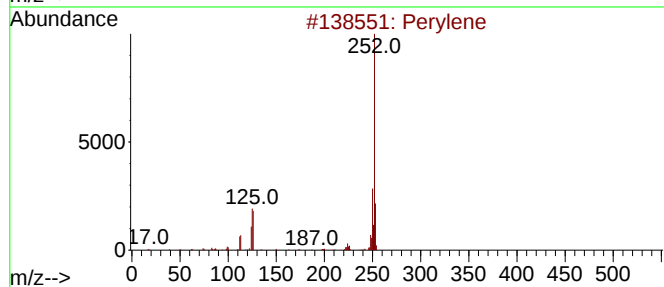
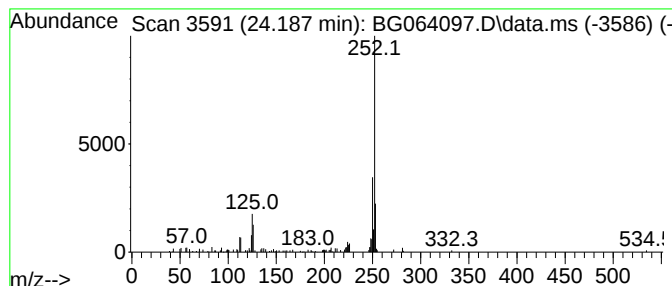
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.187	4.62 ng	168067	Perylene-d12	24.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	96
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
4			Benzo[a]pyrene	252	C20H12	000050-32-8	89
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
Data File : BG064097.D
Acq On : 11 Mar 2025 15:56
Operator : RC/JU
Sample : Q1534-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-18

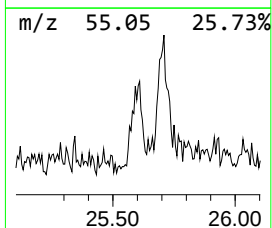
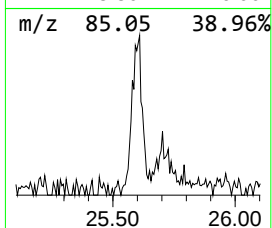
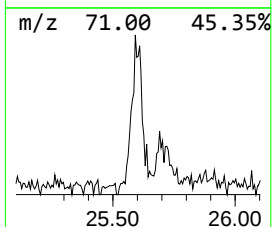
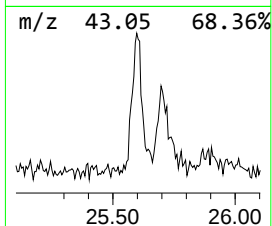
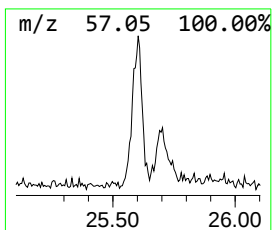
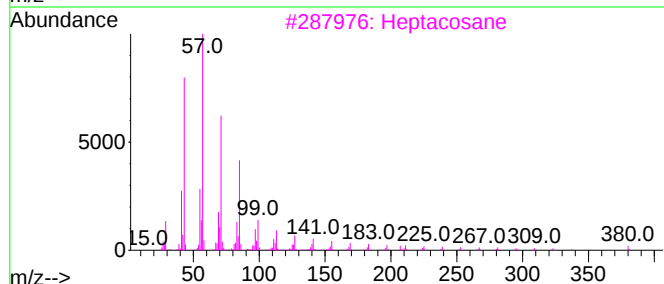
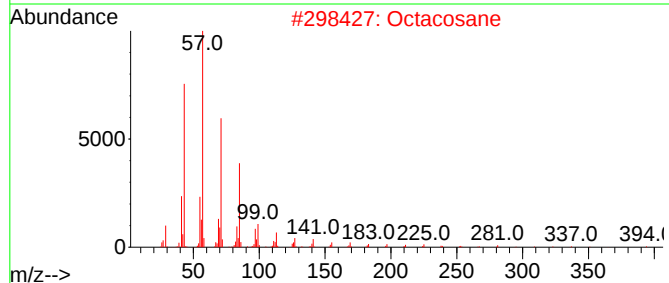
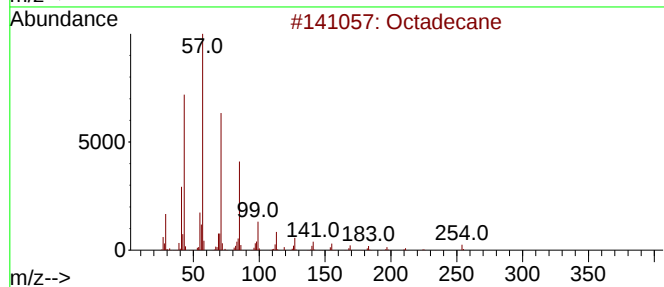
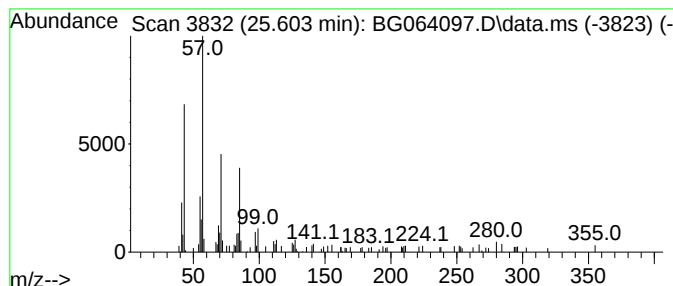
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.603	2.96 ng	107854	Perylene-d12	24.475

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	93
2		Octacosane	394	C28H58	000630-02-4	87
3		Heptacosane	380	C27H56	000593-49-7	83
4		Tetracosane	338	C24H50	000646-31-1	83
5		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
Data File : BG064097.D
Acq On : 11 Mar 2025 15:56
Operator : RC/JU
Sample : Q1534-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-18

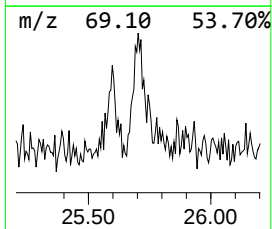
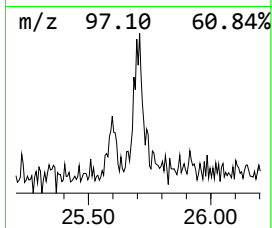
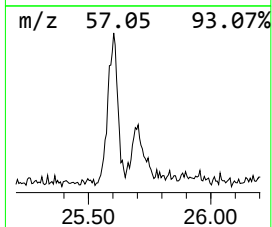
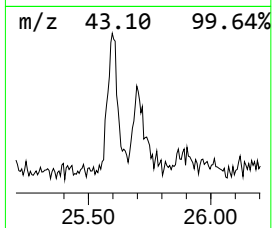
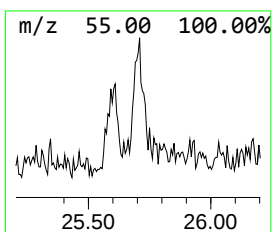
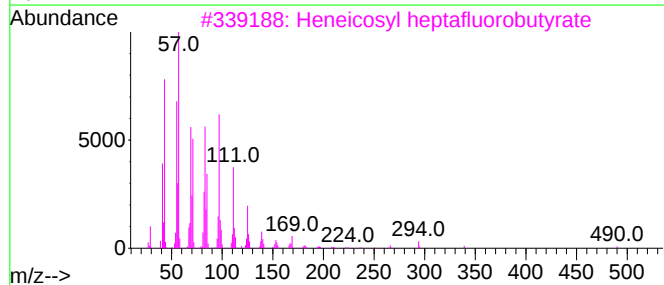
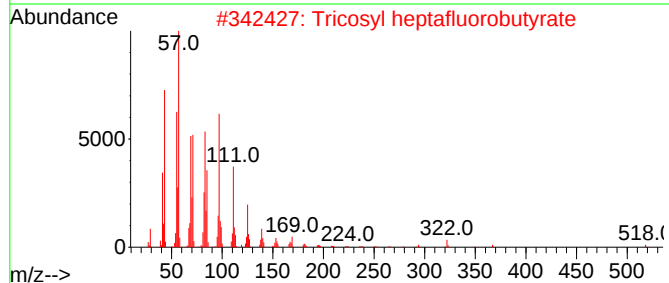
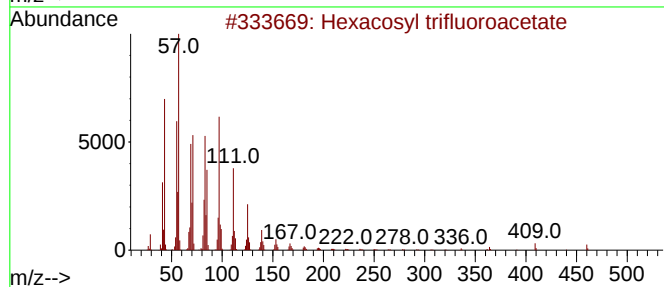
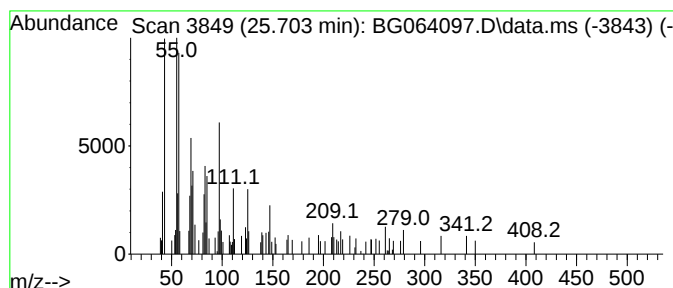
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.703	2.46 ng	89530	Perylene-d12	24.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	64
2			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	64
3			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	64
4			Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	64
5			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031125\
Data File : BG064097.D
Acq On : 11 Mar 2025 15:56
Operator : RC/JU
Sample : Q1534-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-363-COMP-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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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Benzophenone	15.844	11.8	ng	300069	3	14.487	506742	20.0
n-Hexadecanoic ...	18.135	15.4	ng	468434	4	17.225	609937	20.0
1,6-Methano-1H-...	18.500	3.1	ng	95698	4	17.225	609937	20.0
Octadecanoic acid	19.404	2.0	ng	99679	5	21.455	975562	20.0
Cyclohexadecane	21.138	6.0	ng	293308	5	21.455	975562	20.0
Perylene	24.187	4.6	ng	168067	6	24.475	727948	20.0
Octadecane	25.603	3.0	ng	107854	6	24.475	727948	20.0
Hexacosyl trifl...	25.703	2.5	ng	89530	6	24.475	727948	20.0