

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091925\
 Data File : BP025797.D
 Acq On : 19 Sep 2025 13:43
 Operator : CG/JU
 Sample : Q3083-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW3S

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_P\Methods\8270E-BP091225.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025797.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.014	8	13	29	rVB	5383191	6425963	58.62%	10.173%
2	3.308	59	63	71	rVB	80962	110963	1.01%	0.176%
3	4.908	329	335	348	rVB3	59586	114751	1.05%	0.182%
4	5.378	409	415	434	rBV	1604428	2615535	23.86%	4.141%
5	6.943	671	681	694	rBV	926128	1801509	16.43%	2.852%
6	7.749	811	818	827	rBV	634113	1019193	9.30%	1.613%
7	8.896	1005	1013	1026	rBV	2040225	3561207	32.48%	5.638%
8	10.519	1281	1289	1304	rBV	753558	1383554	12.62%	2.190%
9	12.337	1590	1598	1604	rVB2	63457	111574	1.02%	0.177%
10	12.984	1699	1708	1726	rBV	4824256	7937653	72.41%	12.566%
11	13.654	1817	1822	1827	rBV2	78102	120068	1.10%	0.190%
12	14.372	1937	1944	1950	rBV	1139852	1860086	16.97%	2.945%
13	14.437	1950	1955	1965	rVB	472567	718568	6.55%	1.138%
14	14.813	2014	2019	2031	rBV2	93504	188274	1.72%	0.298%
15	15.354	2107	2111	2119	rBV	133937	227002	2.07%	0.359%
16	15.437	2121	2125	2131	rVB2	81810	129280	1.18%	0.205%
17	15.754	2173	2179	2186	rBV	361407	509667	4.65%	0.807%
18	15.890	2195	2202	2213	rBV	3821980	6125135	55.87%	9.696%
19	16.101	2234	2238	2250	rVB	118757	215729	1.97%	0.342%
20	16.578	2316	2319	2324	rVB	91568	113831	1.04%	0.180%
21	17.172	2414	2420	2426	rBV2	1393022	2185473	19.94%	3.460%
22	17.454	2463	2468	2478	rBV	2353025	3273756	29.86%	5.183%
23	17.984	2553	2558	2568	rBV	229714	424849	3.88%	0.673%
24	18.113	2575	2580	2588	rBV	1699919	2480387	22.63%	3.927%
25	19.313	2779	2784	2800	rVB2	228262	522576	4.77%	0.827%
26	19.448	2802	2807	2820	rBV	627242	1059966	9.67%	1.678%
27	19.901	2878	2884	2891	rBV	8027789	10962641	100.00%	17.354%
28	20.172	2927	2930	2935	rBV	83306	121129	1.10%	0.192%
29	21.289	3116	3120	3128	rBV	410589	677753	6.18%	1.073%
30	21.630	3172	3178	3185	rBV	1526028	2461971	22.46%	3.897%
31	23.442	3480	3486	3495	rVB	678864	1317520	12.02%	2.086%
32	24.989	3741	3749	3762	rVB	900797	2391813	21.82%	3.786%

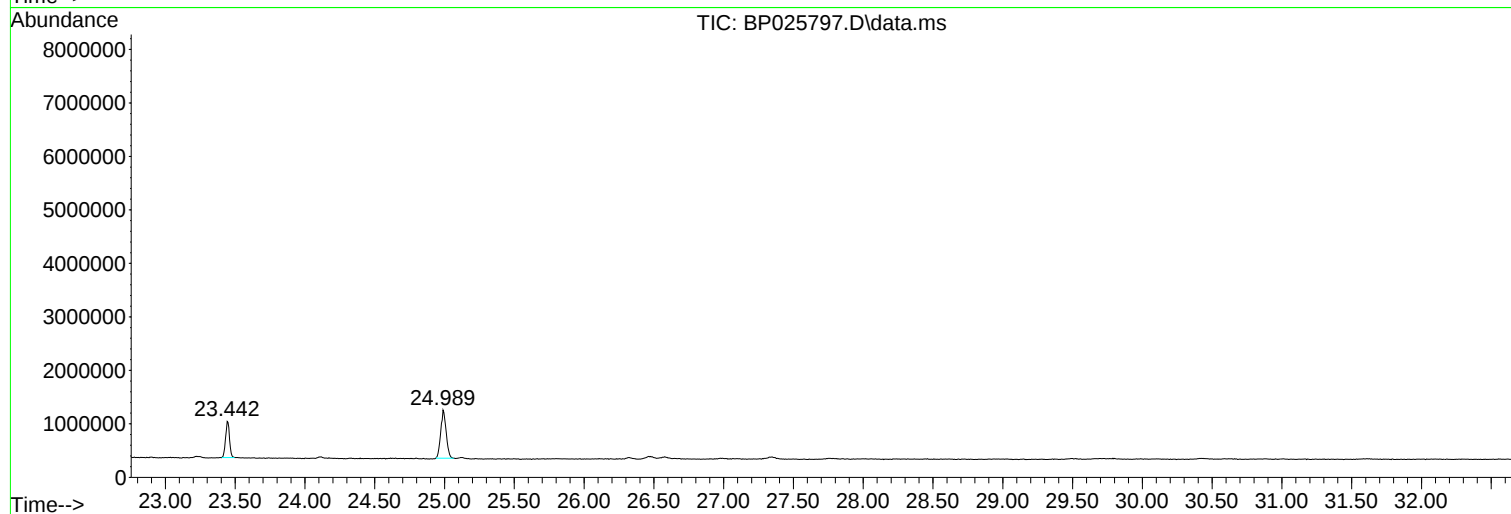
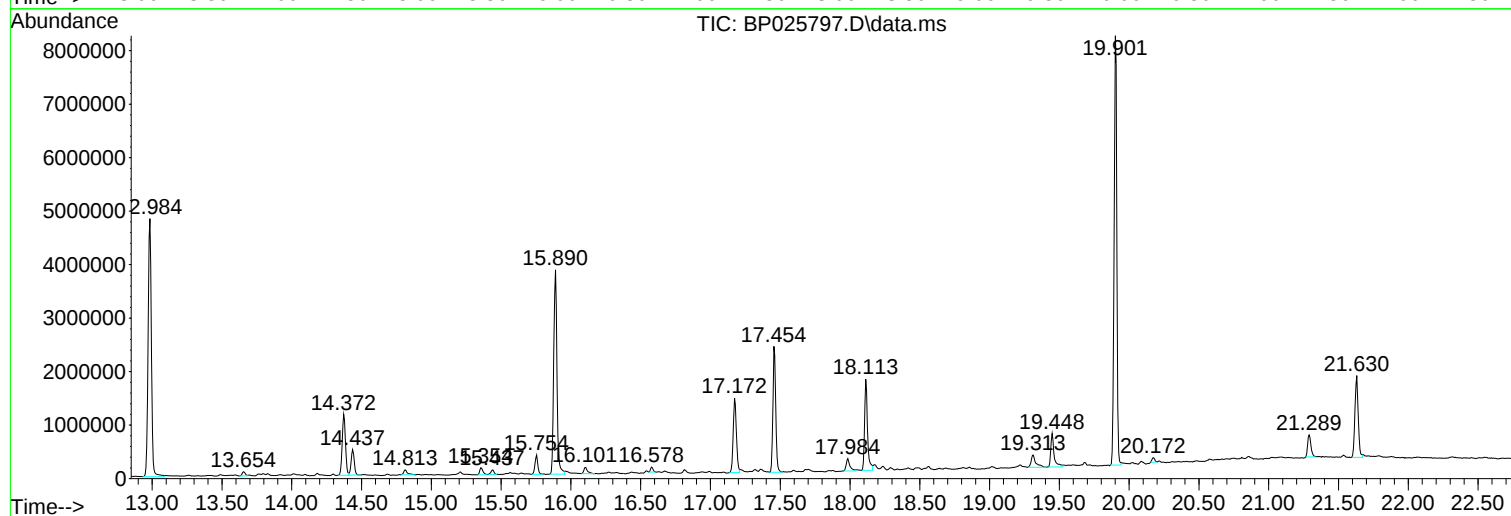
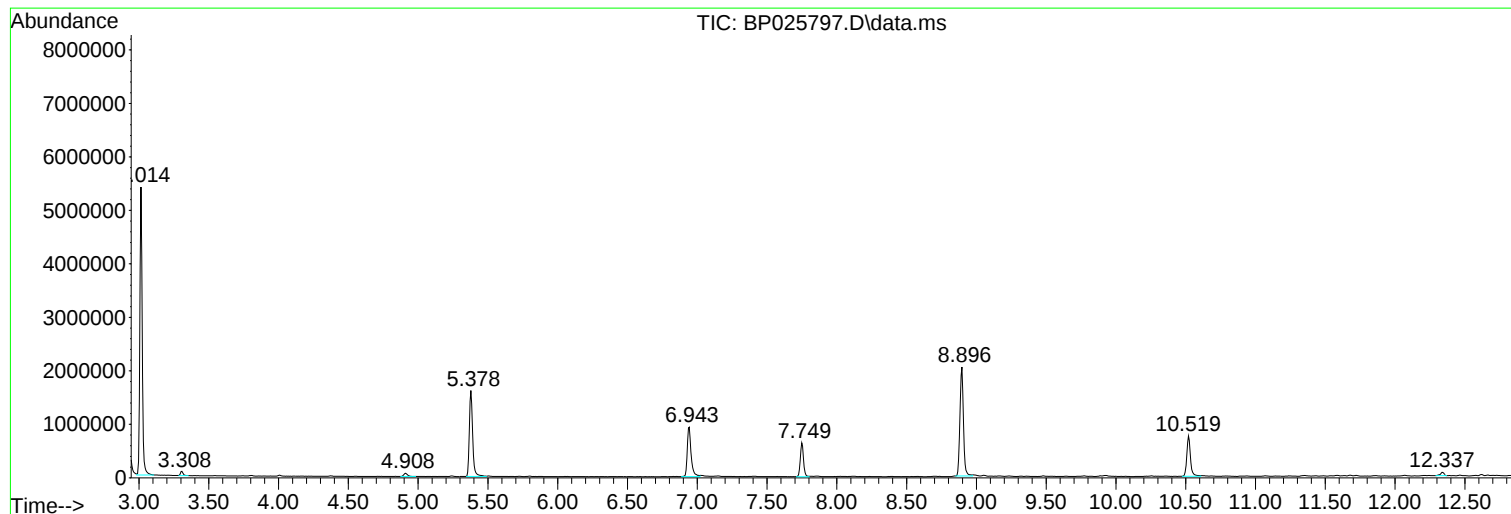
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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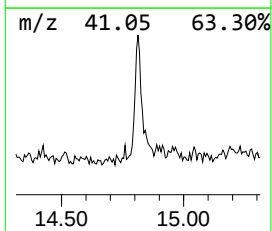
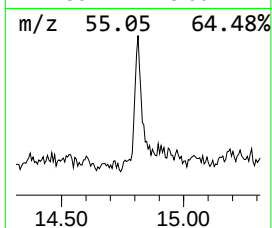
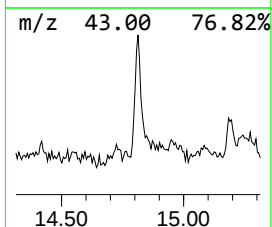
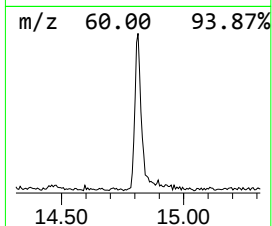
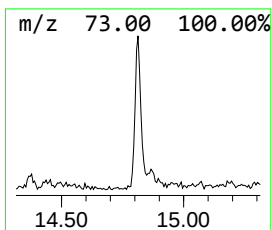
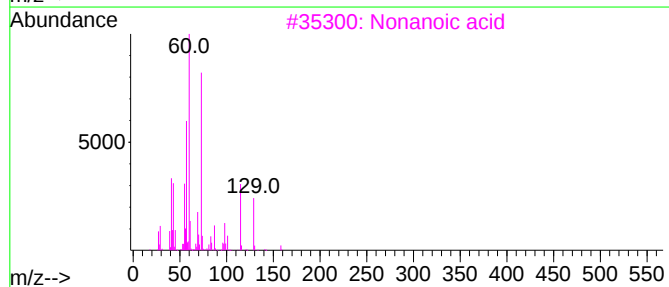
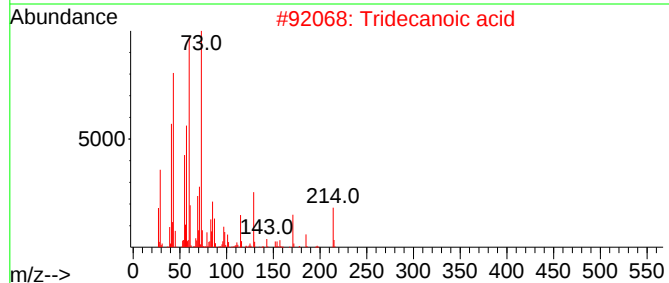
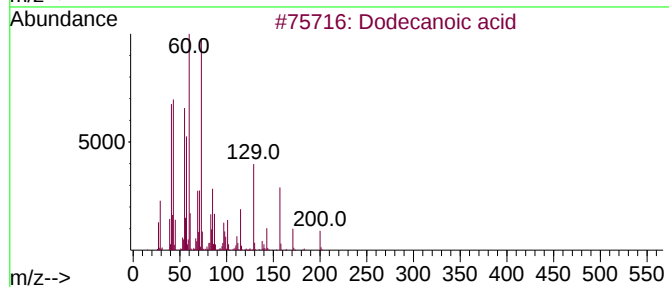
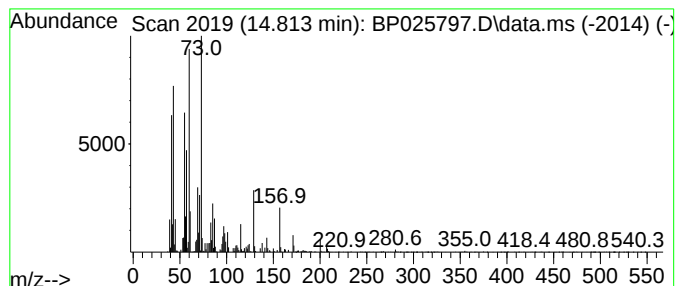
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BNA_P
ClientSampleId :
MW3S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Dodecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.813	2.02 ng	188274	Acenaphthene-d10		14.372	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecanoic acid		200	C12H24O2	000143-07-7	93
2	Tridecanoic acid		214	C13H26O2	000638-53-9	87
3	Nonanoic acid		158	C9H18O2	000112-05-0	64
4	n-Decanoic acid		172	C10H20O2	000334-48-5	58
5	Octanoic acid		144	C8H16O2	000124-07-2	52



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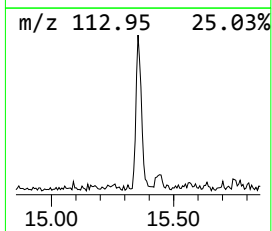
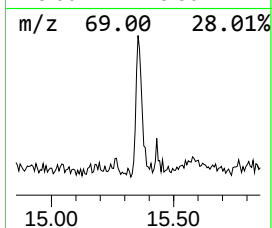
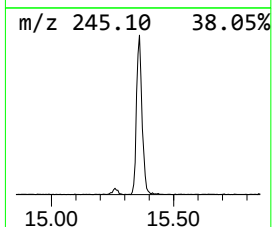
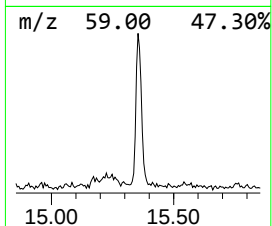
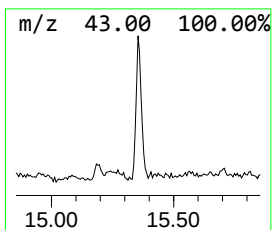
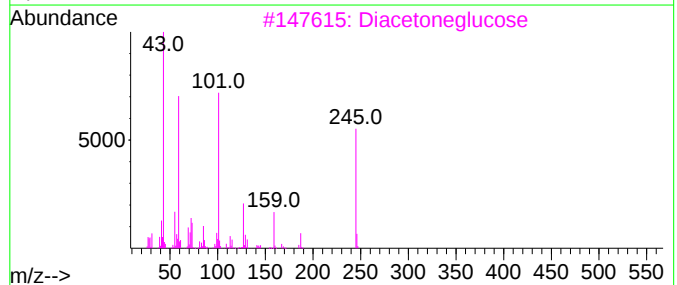
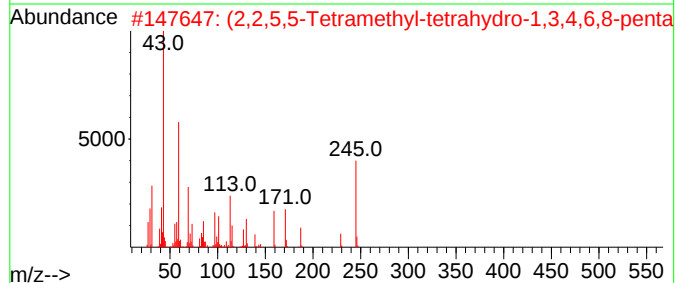
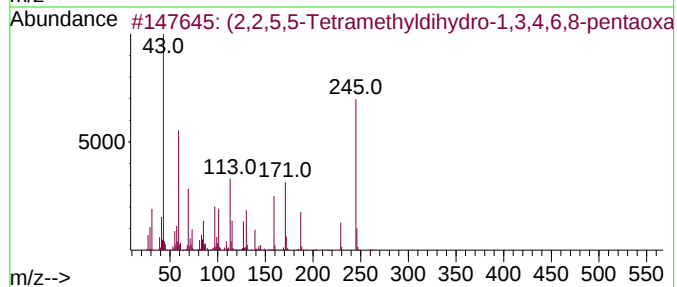
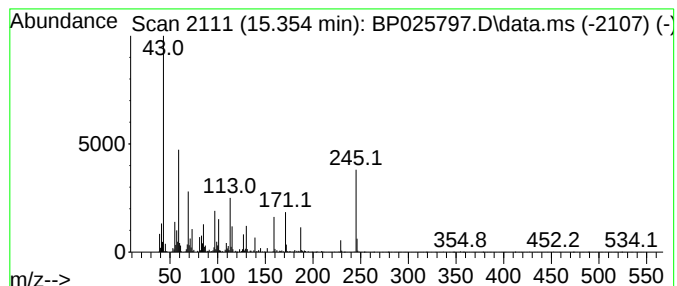
Instrument :
BNA_P
ClientSampleId :
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TIC Integration Parameters: LSCINT.P

Peak Number 4 (2,2,5,5-Tetramethyldihydro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.354	2.44 ng	227002	Acenaphthene-d10	14.372	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,2,5,5-Tetramethyldihydro-1,3,...	260	C12H20O6	1000192-04-6	98
2	(2,2,5,5-Tetramethyl-tetrahydro-...	260	C12H20O6	1000193-90-4	91
3	Diacetoneglucose	260	C12H20O6	000582-52-5	38
4	.alpha.-D-Galactopyranose, 1,2:3...	260	C12H20O6	004064-06-6	30
5	Diisopropylidene l-idose	260	C12H20O6	1000127-52-3	25



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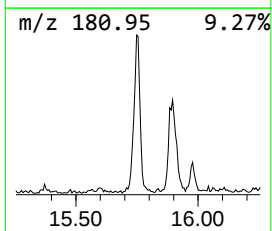
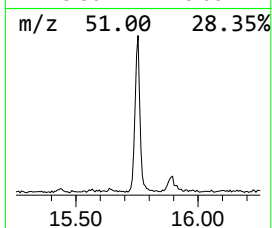
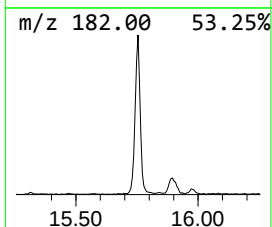
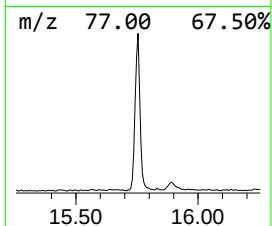
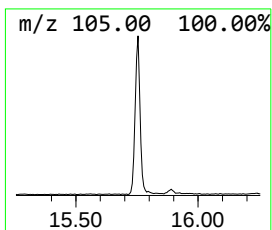
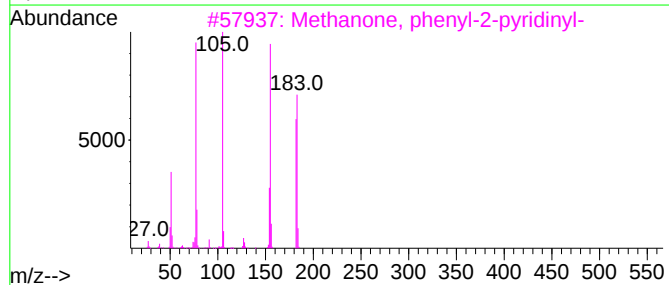
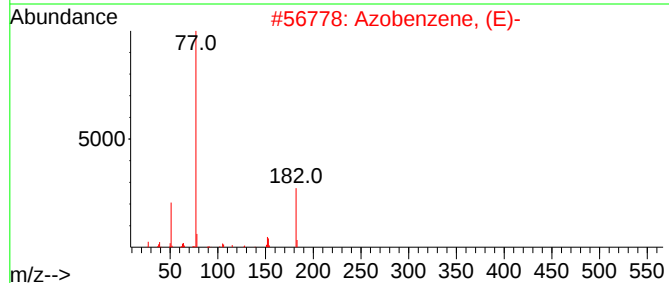
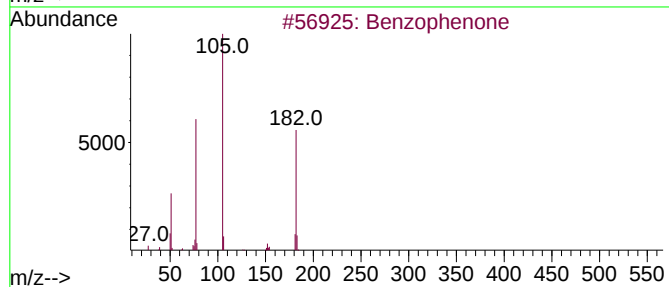
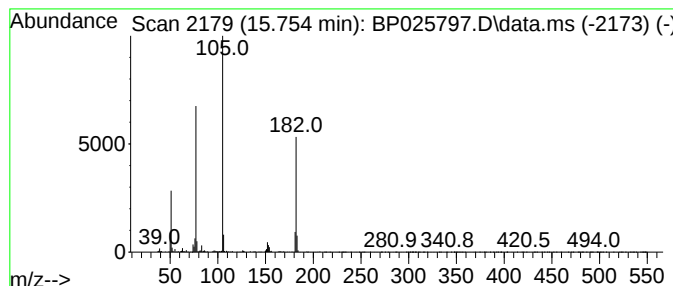
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Peak Number 5 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.754	5.48 ng	509667	Acenaphthene-d10	14.372

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	58
3			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
4			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	42
5			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	40



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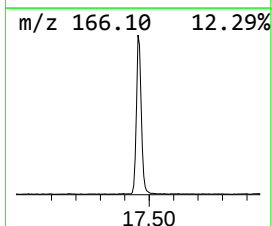
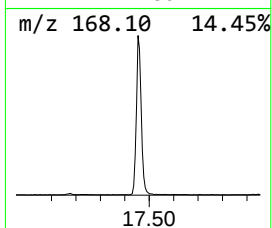
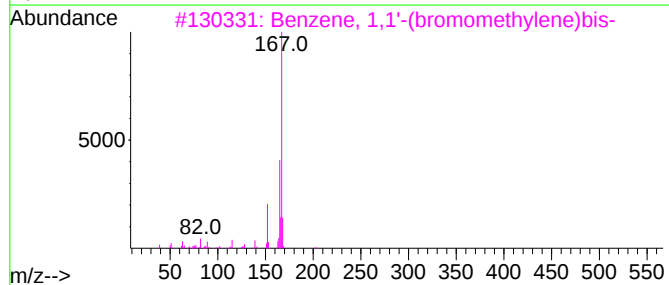
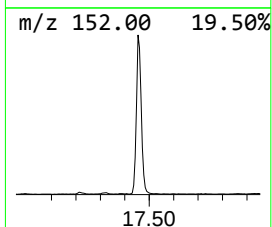
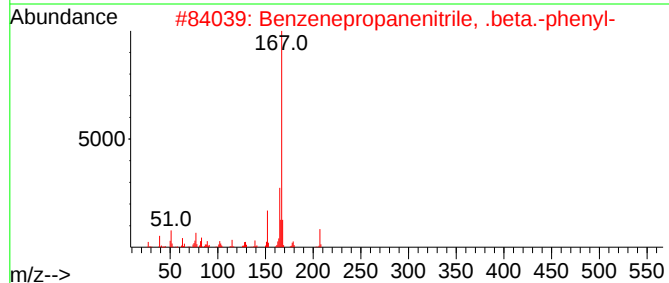
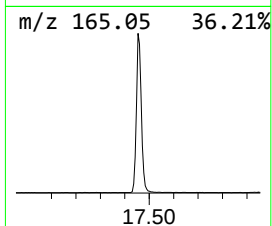
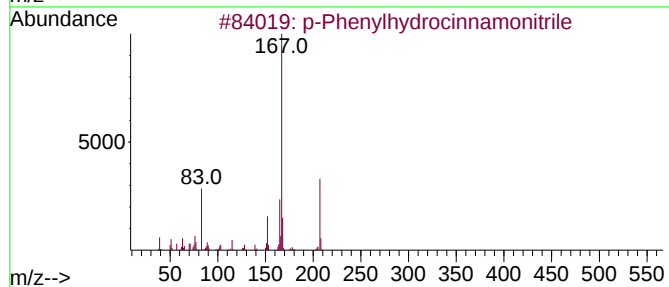
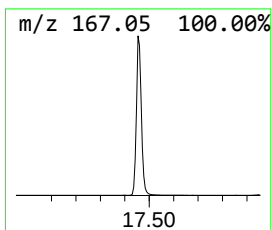
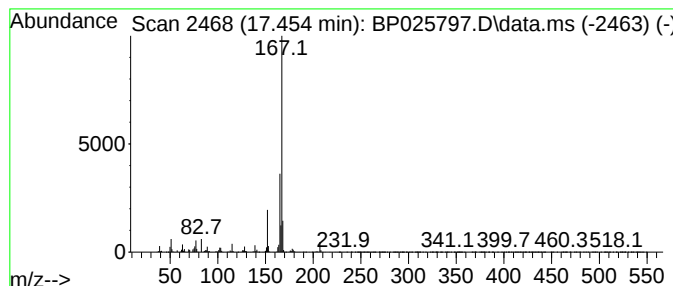
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Peak Number 6 p-Phenylhydrocinnamonitrile Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.454	29.96 ng	3273760	Phenanthrene-d10	17.172	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Phenylhydrocinnamonitrile	207	C15H13N	092552-19-7	91
2	Benzenepropanenitrile, .beta.-ph...	207	C15H13N	002286-54-6	91
3	Benzene, 1,1'-(bromomethylene)bis-	246	C13H11Br	000776-74-9	87
4	Adrafinil	289	C15H15NO3S	063547-13-7	87
5	2-Propanone, 1,1-diphenyl-	210	C15H14O	000781-35-1	87



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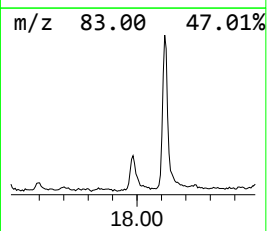
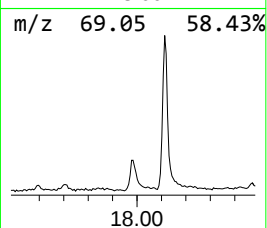
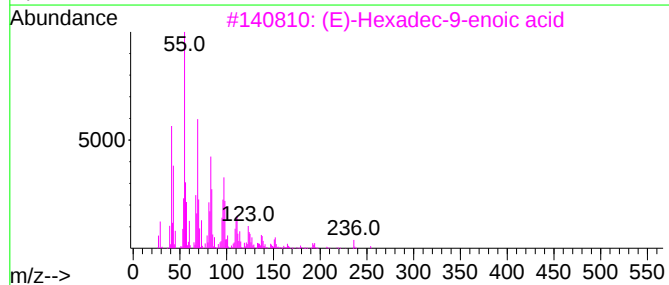
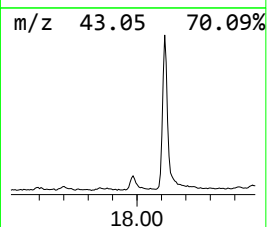
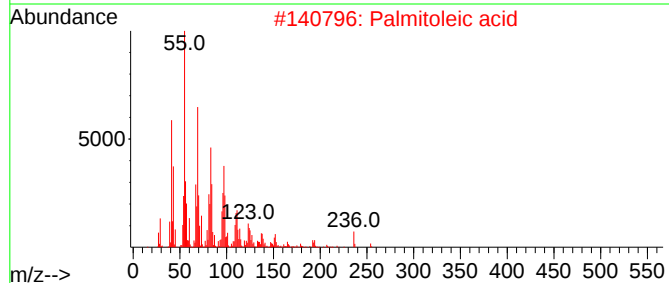
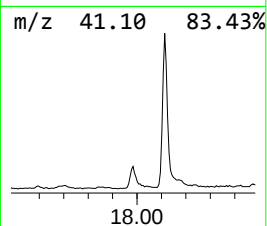
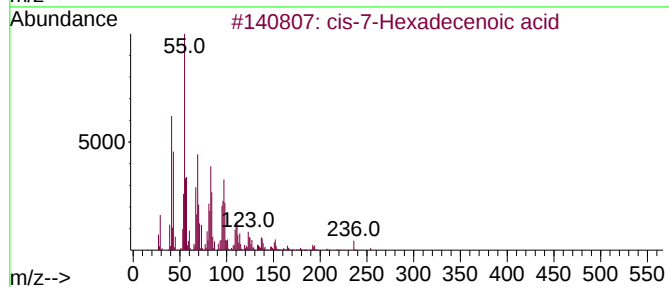
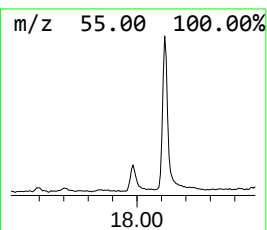
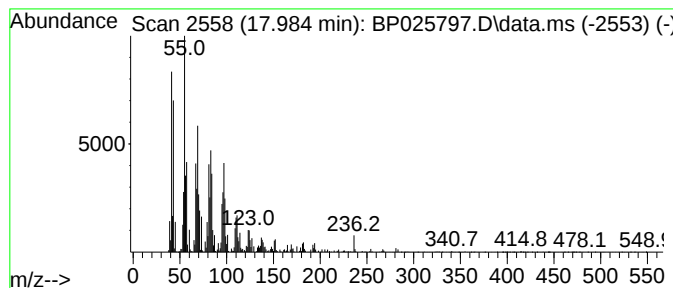
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Peak Number 7 cis-7-Hexadecenoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.984	3.89 ng	424849	Phenanthrene-d10	17.172

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
2			Palmitoleic acid	254	C16H30O2	000373-49-9	98
3			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	98
4			7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	93
5			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	90



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ALS Vial : 7 Sample Multiplier: 1

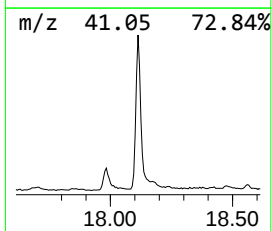
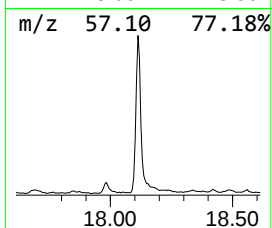
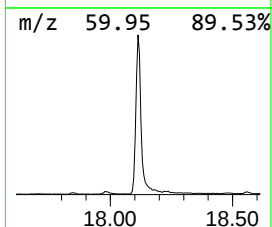
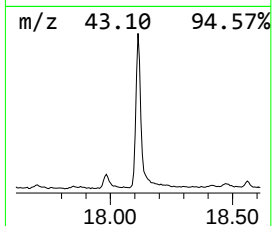
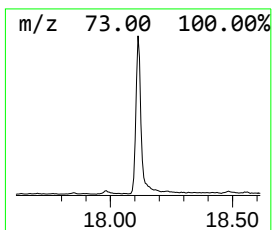
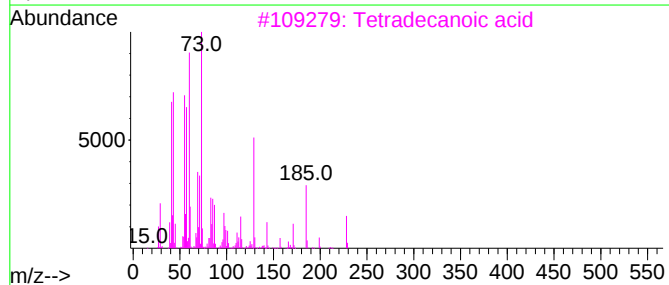
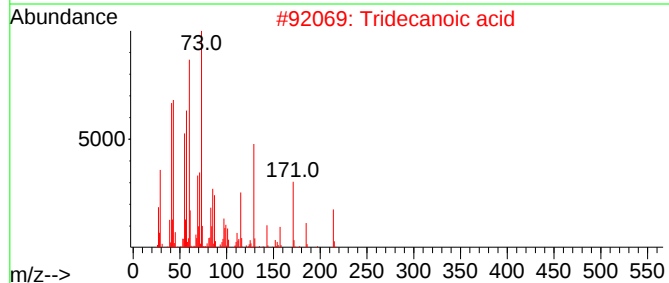
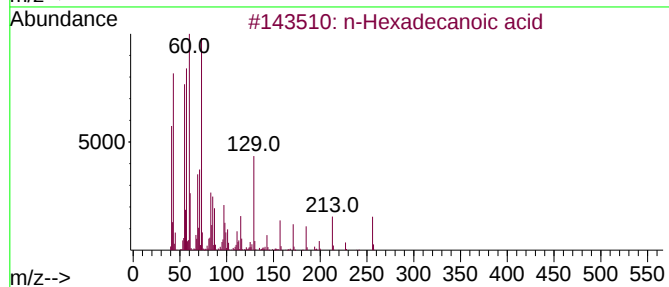
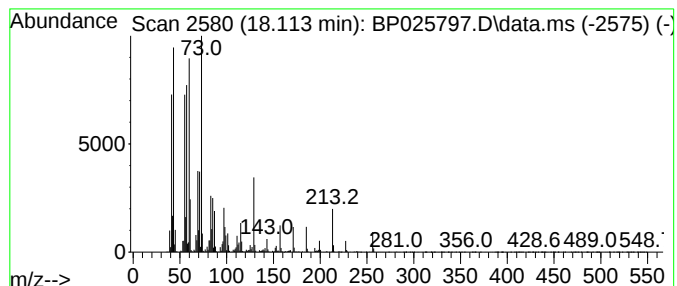
Instrument :
BNA_P
ClientSampleId :
MW3S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.113	22.70 ng	2480390	Phenanthrene-d10		17.172	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	83
5	Nonanoic acid		158	C9H18O2	000112-05-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091925\
Data File : BP025797.D
Acq On : 19 Sep 2025 13:43
Operator : CG/JU
Sample : Q3083-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW3S

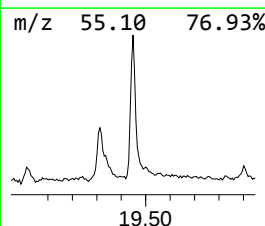
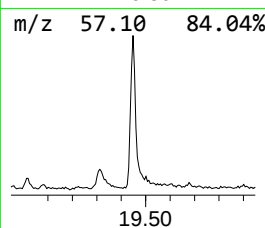
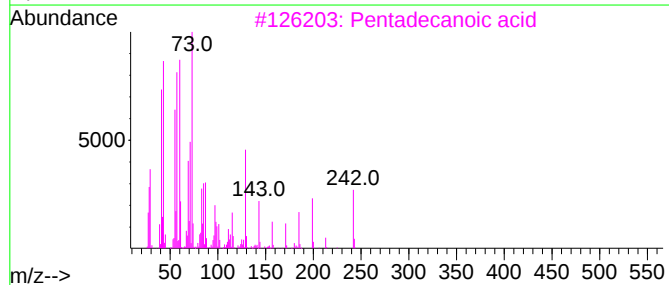
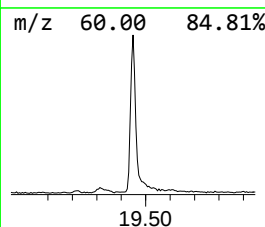
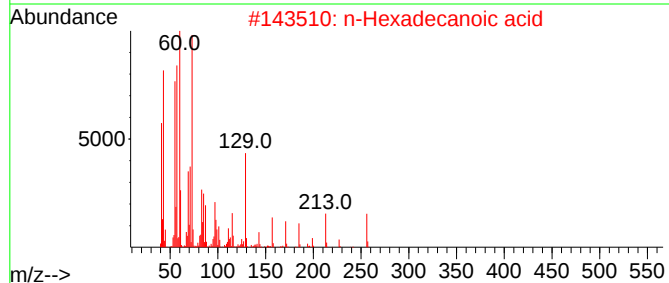
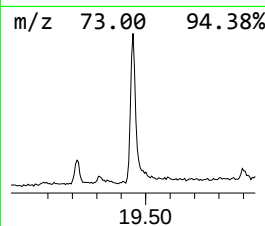
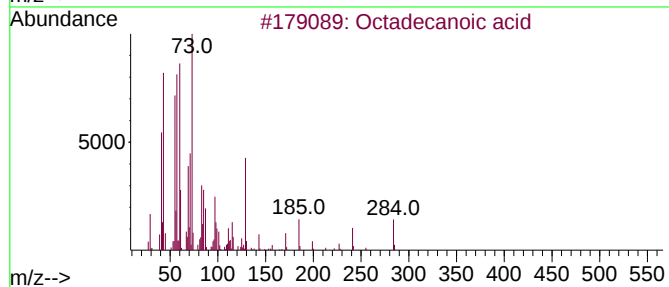
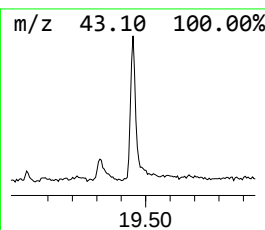
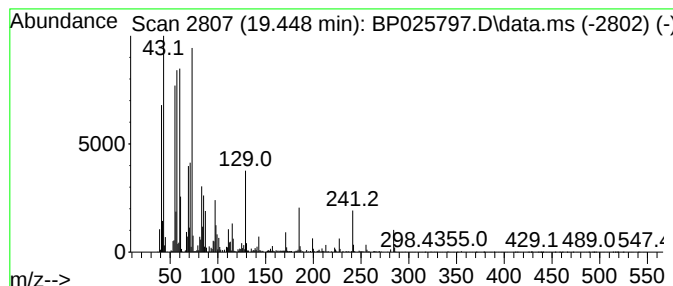
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.448	8.61 ng	1059970	Chrysene-d12	21.631

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091925\
Data File : BP025797.D
Acq On : 19 Sep 2025 13:43
Operator : CG/JU
Sample : Q3083-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

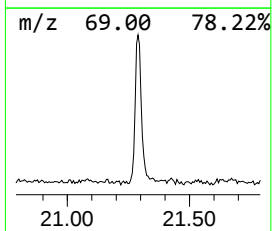
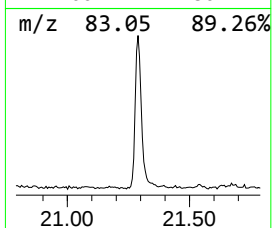
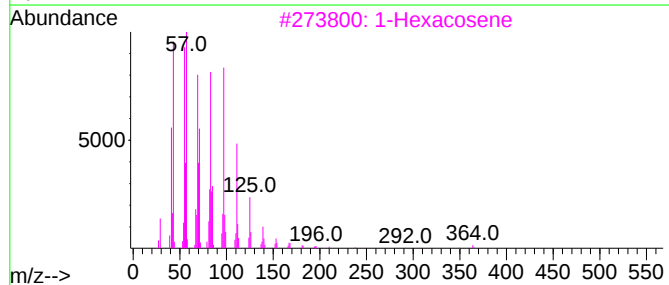
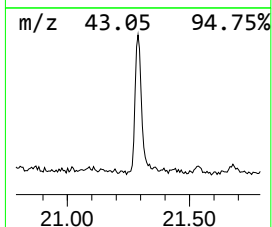
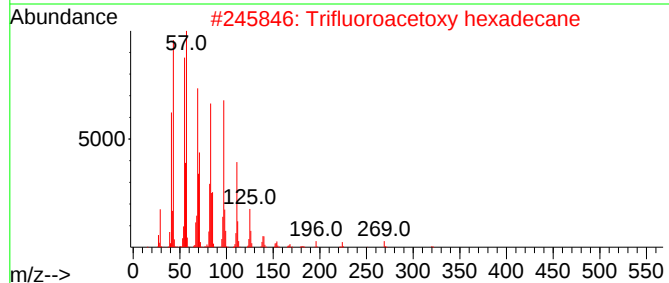
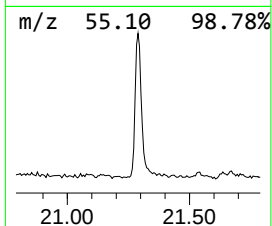
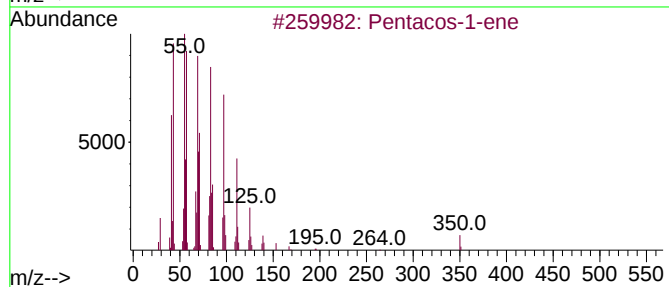
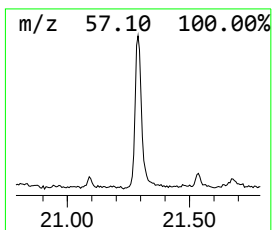
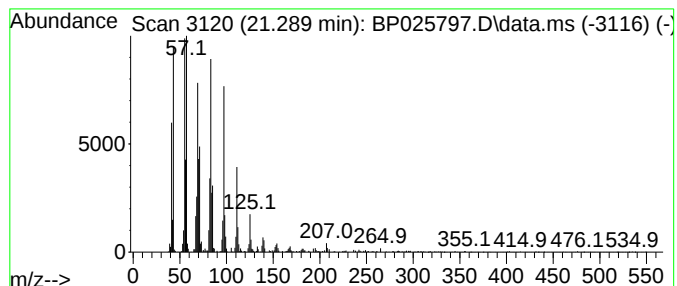
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacos-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.289	5.51 ng	677753	Chrysene-d12		21.631	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentacos-1-ene		350	C25H50	016980-85-1	94
2	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
3	1-Hexacosene		364	C26H52	018835-33-1	94
4	1-Heneicosyl formate		340	C22H44O2	077899-03-7	94
5	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091925\
Data File : BP025797.D
Acq On : 19 Sep 2025 13:43
Operator : CG/JU
Sample : Q3083-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW3S

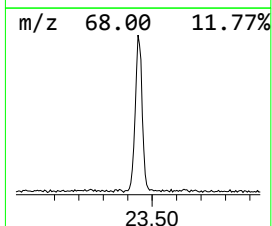
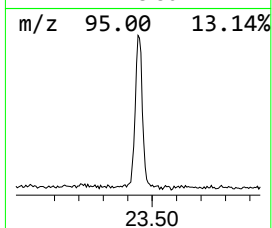
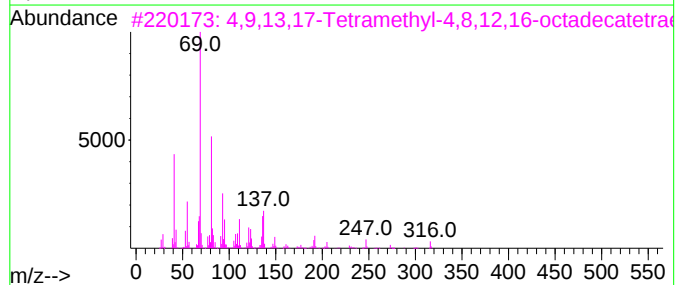
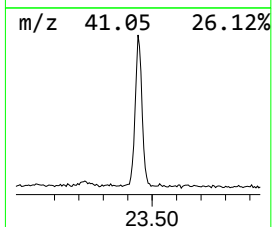
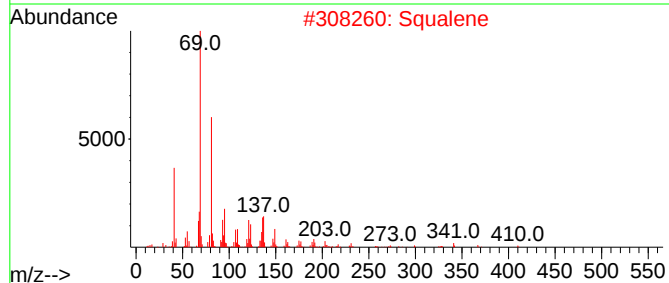
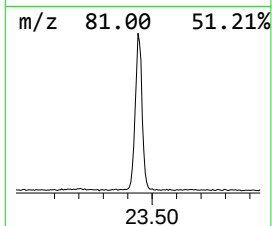
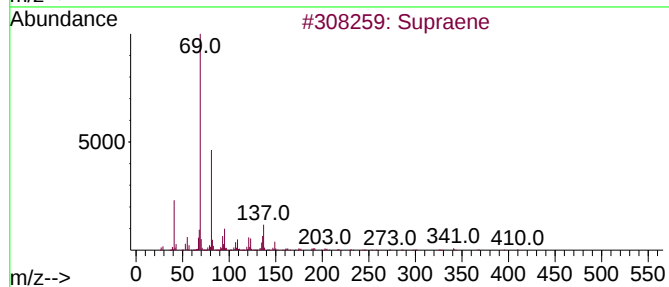
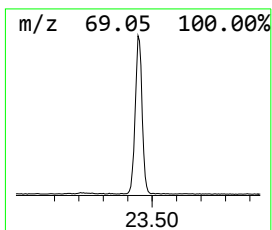
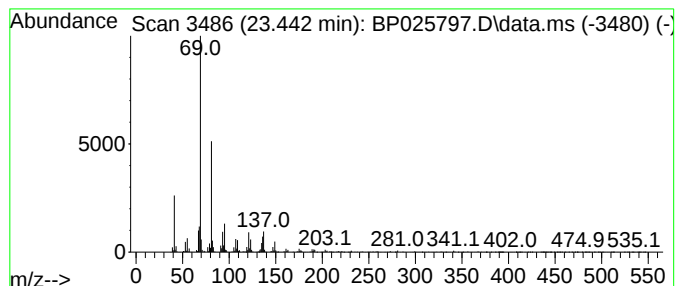
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.442	11.02 ng	1317520	Perylene-d12	24.989

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	90
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091925\
Data File : BP025797.D
Acq On : 19 Sep 2025 13:43
Operator : CG/JU
Sample : Q3083-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW3S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dodecanoic acid	14.813	2.0	ng	188274	3	14.372	1860090	20.0
(2,2,5,5-Tetram...	15.354	2.4	ng	227002	3	14.372	1860090	20.0
Benzophenone	15.754	5.5	ng	509667	3	14.372	1860090	20.0
p-Phenylhydroci...	17.454	30.0	ng	3273760	4	17.172	2185470	20.0
cis-7-Hexadecen...	17.984	3.9	ng	424849	4	17.172	2185470	20.0
n-Hexadecanoic ...	18.113	22.7	ng	2480390	4	17.172	2185470	20.0
Octadecanoic acid	19.448	8.6	ng	1059970	5	21.631	2461970	20.0
Pentacos-1-ene	21.289	5.5	ng	677753	5	21.631	2461970	20.0
Supraene	23.442	11.0	ng	1317520	6	24.989	2391810	20.0