

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061225\
 Data File : BP024935.D
 Acq On : 12 Jun 2025 18:37
 Operator : RC/JU
 Sample : Q2297-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-3

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-BP060625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024935.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.772	307	312	321	rBV	283112	386189	4.33%	0.634%
2	5.237	385	391	409	rBV	2903856	4479673	50.19%	7.349%
3	6.813	652	659	678	rBV	2639707	4727129	52.96%	7.755%
4	7.608	786	794	803	rBV	865124	1349630	15.12%	2.214%
5	8.760	982	990	1006	rBV	1836387	3059179	34.28%	5.019%
6	10.378	1256	1265	1280	rBV	1099312	1895442	21.24%	3.109%
7	12.854	1675	1686	1704	rBV	4363004	6532668	73.19%	10.717%
8	13.966	1869	1875	1885	rVB2	61840	129409	1.45%	0.212%
9	14.254	1917	1924	1931	rBV	1557156	2388170	26.76%	3.918%
10	15.642	2153	2160	2172	rBV	1024653	1452184	16.27%	2.382%
11	15.778	2176	2183	2203	rVV	3942871	5774516	64.70%	9.473%
12	16.007	2217	2222	2229	rBV4	66103	146328	1.64%	0.240%
13	16.219	2253	2258	2263	rVB	176050	243772	2.73%	0.400%
14	17.054	2394	2400	2404	rBV2	2000868	2781515	31.17%	4.563%
15	17.095	2404	2407	2414	rVB	390238	555055	6.22%	0.911%
16	17.195	2420	2424	2429	rVB	94563	128695	1.44%	0.211%
17	17.995	2555	2560	2569	rBV2	1214291	1715185	19.22%	2.814%
18	18.160	2584	2588	2592	rBV4	65084	106840	1.20%	0.175%
19	18.289	2608	2610	2621	rVB4	67964	109356	1.23%	0.179%
20	18.442	2631	2636	2639	rBV5	84199	138792	1.56%	0.228%
21	18.730	2681	2685	2690	rVB2	128661	165588	1.86%	0.272%
22	18.889	2708	2712	2720	rVB2	237918	392144	4.39%	0.643%
23	19.189	2757	2763	2768	rBV	918946	1402243	15.71%	2.300%
24	19.325	2782	2786	2793	rBV2	414875	646711	7.25%	1.061%
25	19.530	2818	2821	2822	rBV	114799	117036	1.31%	0.192%
26	19.560	2822	2826	2830	rVV	800400	1058643	11.86%	1.737%
27	19.777	2858	2863	2868	rBV	7304401	8925074	100.00%	14.642%
28	20.083	2912	2915	2919	rBV	306314	367665	4.12%	0.603%
29	21.148	3092	3096	3102	rVB3	785533	1202268	13.47%	1.972%
30	21.483	3147	3153	3158	rBV3	2100959	3655607	40.96%	5.997%
31	21.530	3158	3161	3167	rVB	447338	570523	6.39%	0.936%
32	23.018	3412	3414	3424	rVB2	647048	1079859	12.10%	1.772%
33	24.748	3702	3708	3718	rVB	1330503	3274008	36.68%	5.371%

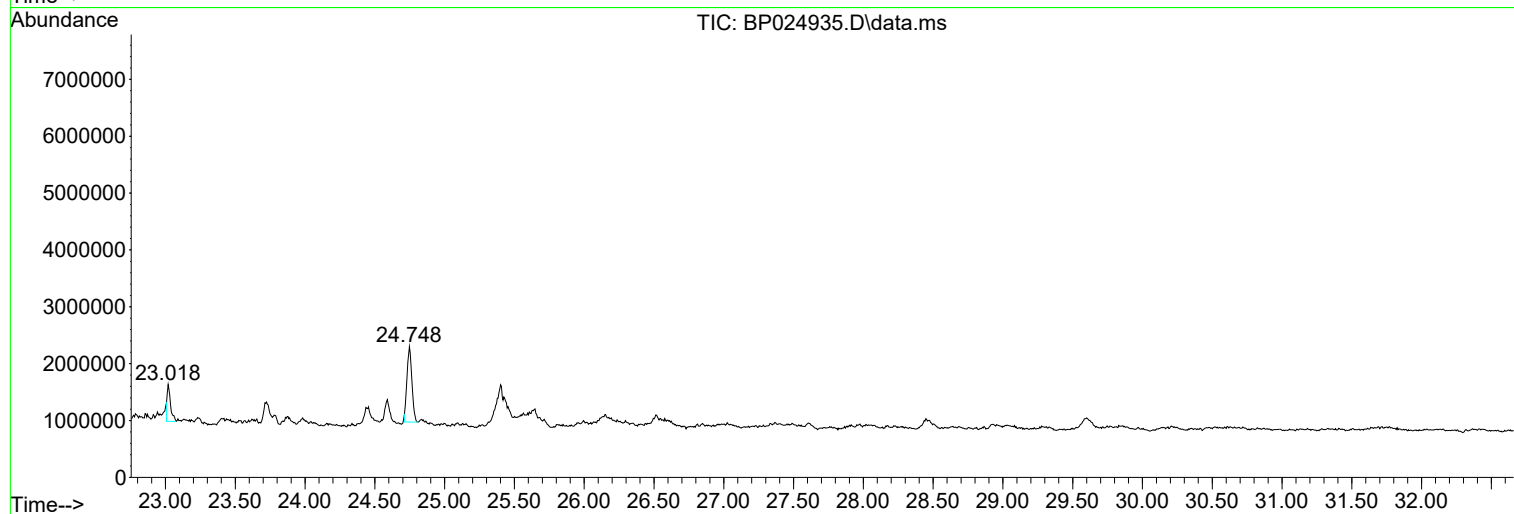
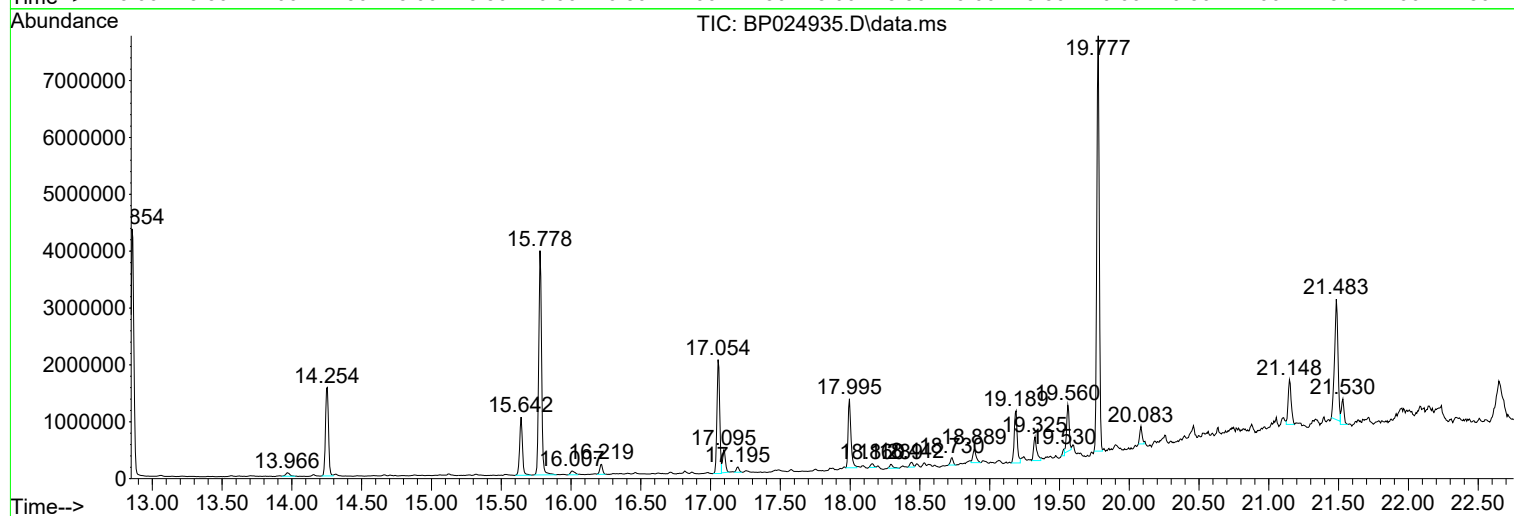
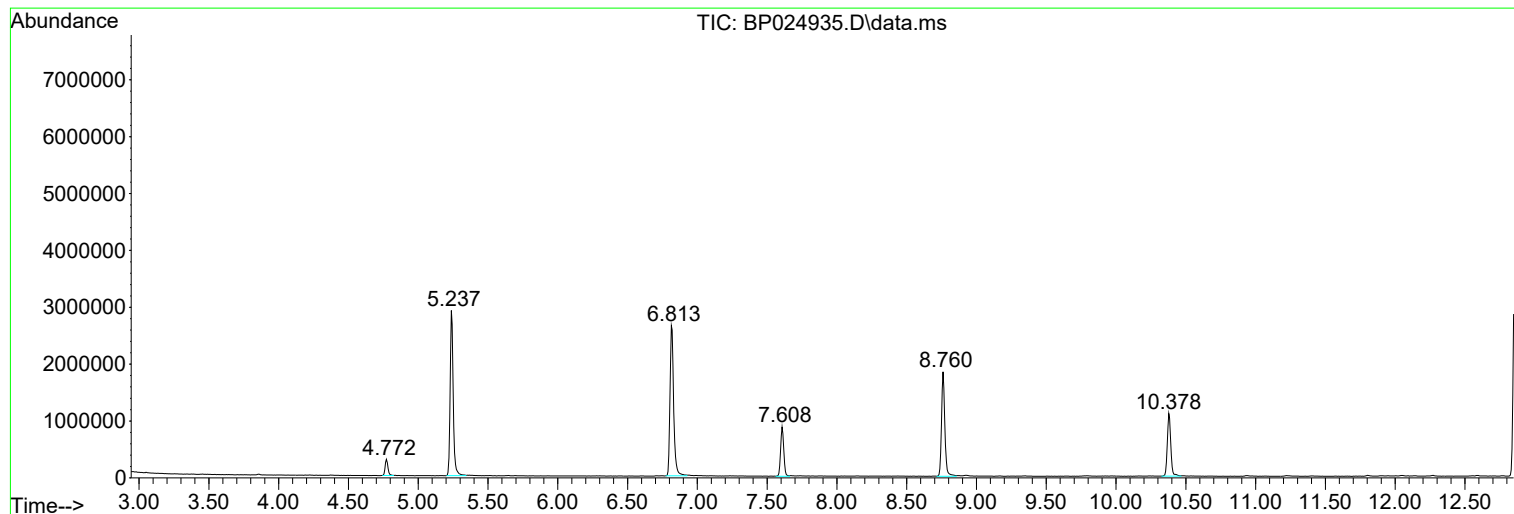
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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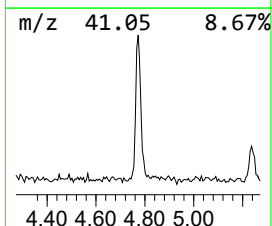
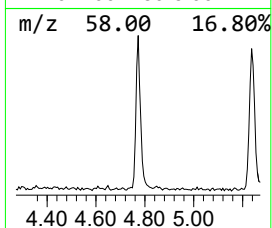
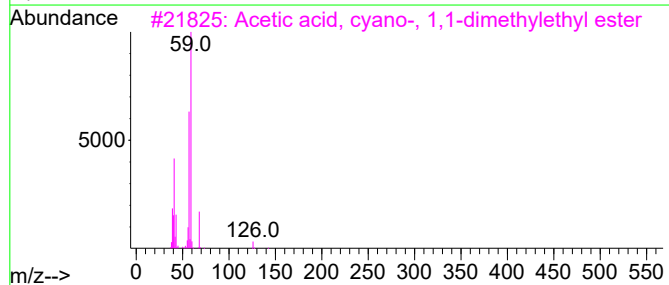
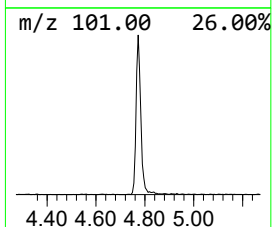
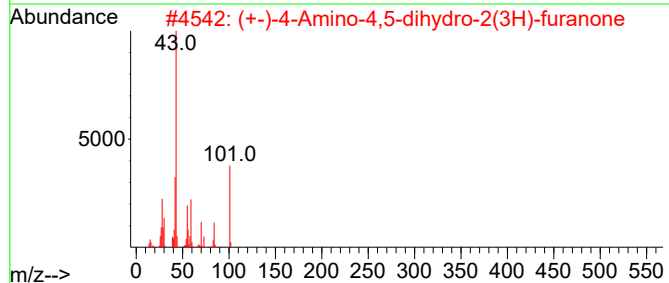
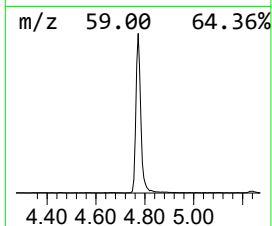
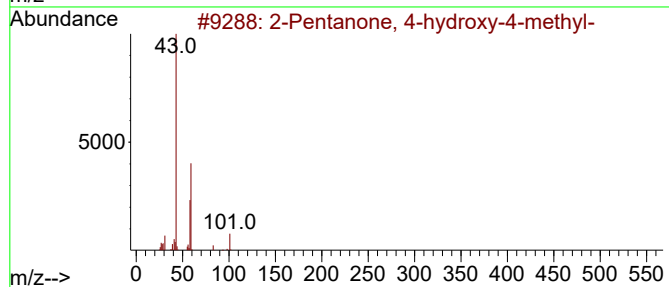
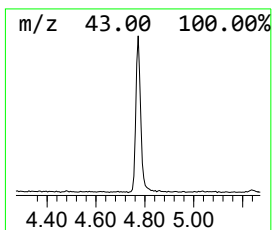
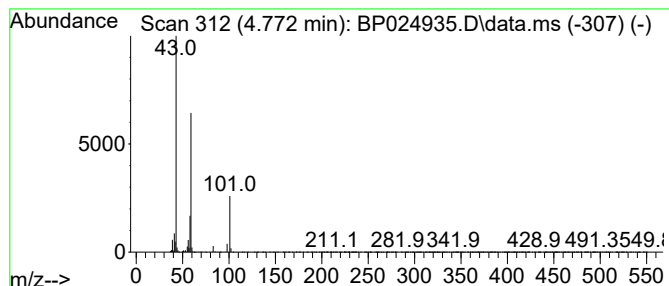
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.772	5.72 ng	386189	1,4-Dichlorobenzene-d4	7.608

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9



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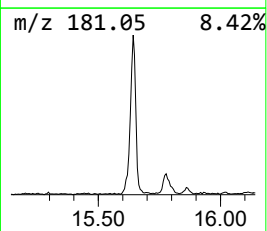
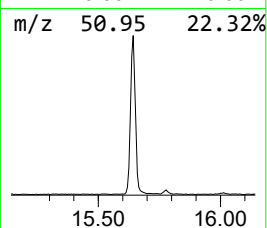
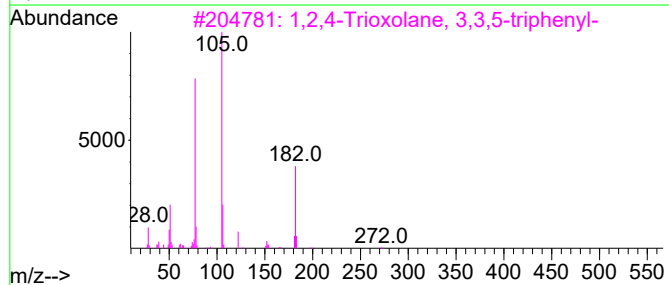
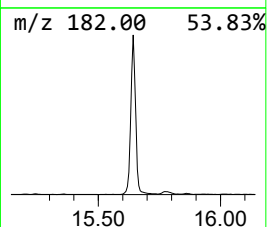
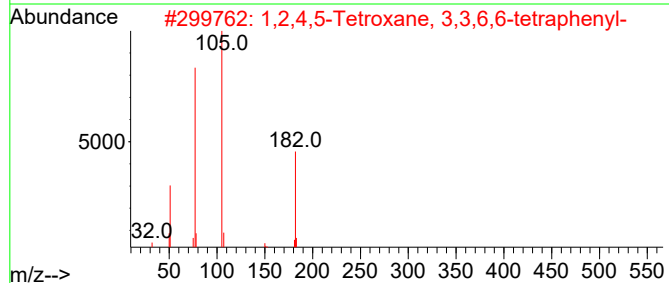
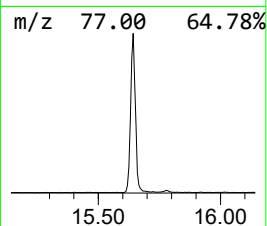
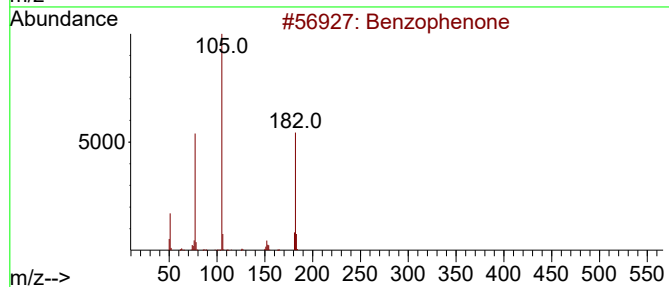
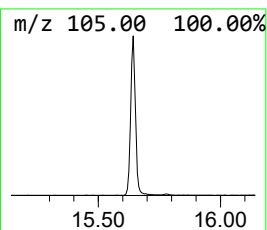
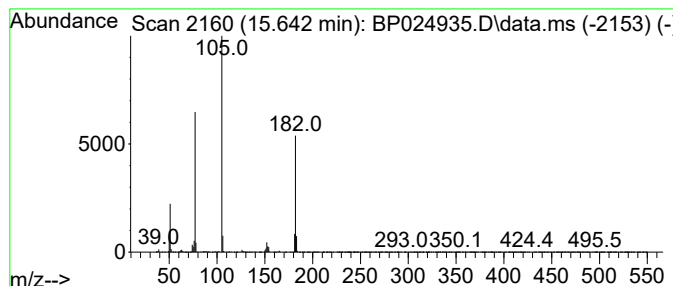
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.642	12.16 ng	1452180	Acenaphthene-d10	14.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	64
3			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50
4			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
5			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45



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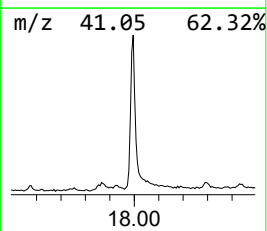
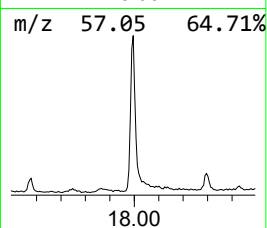
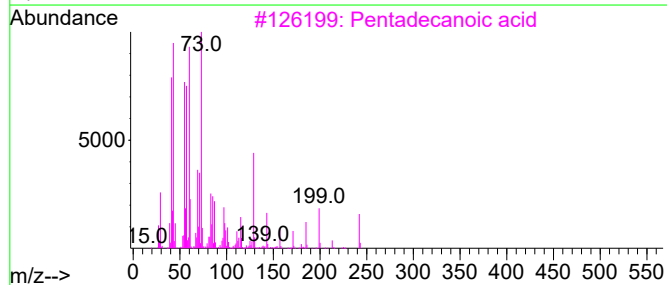
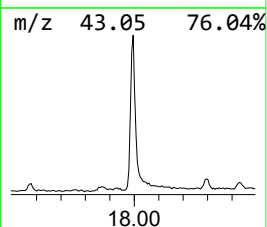
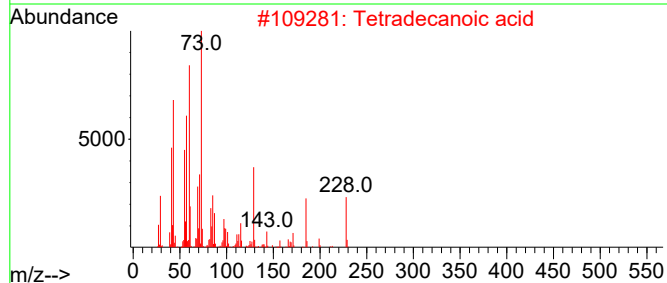
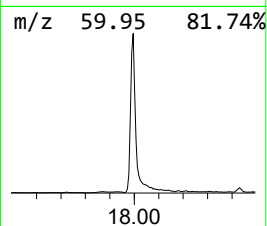
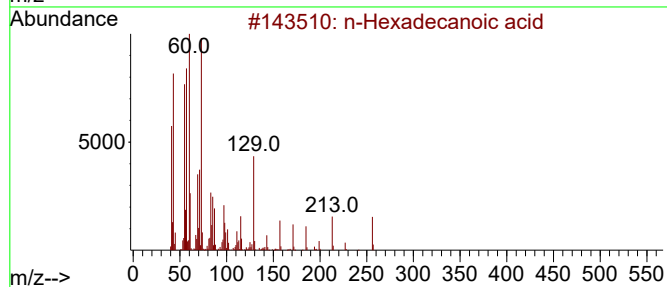
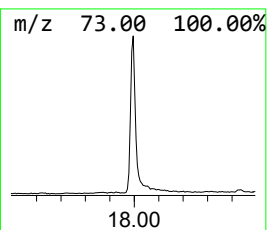
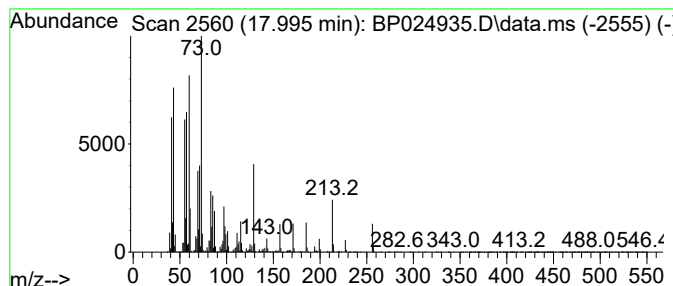
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.995	12.33 ng	1715190	Phenanthrene-d10	17.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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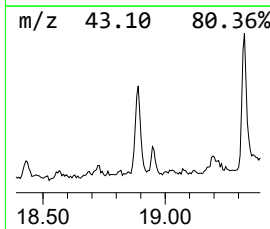
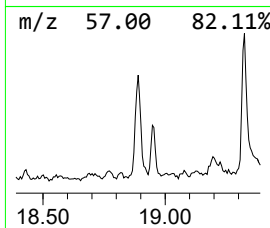
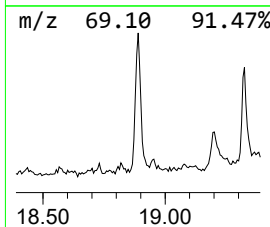
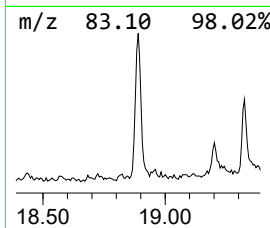
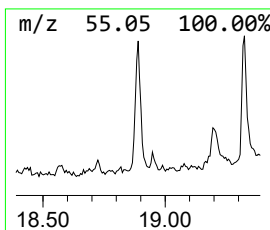
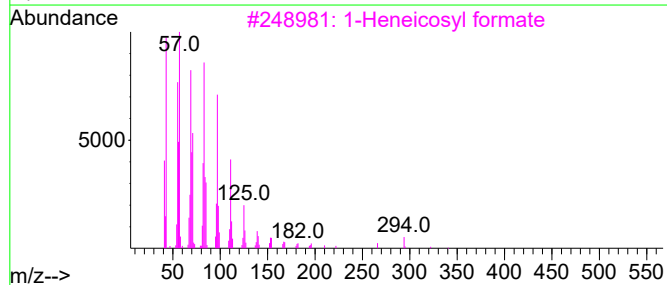
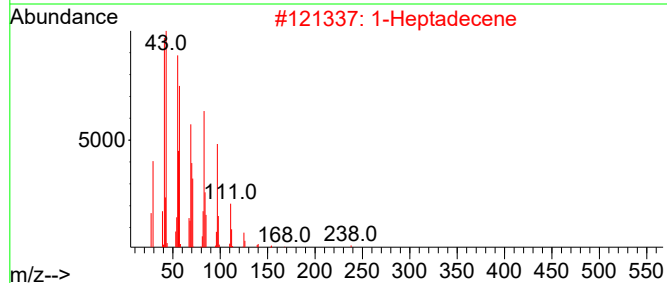
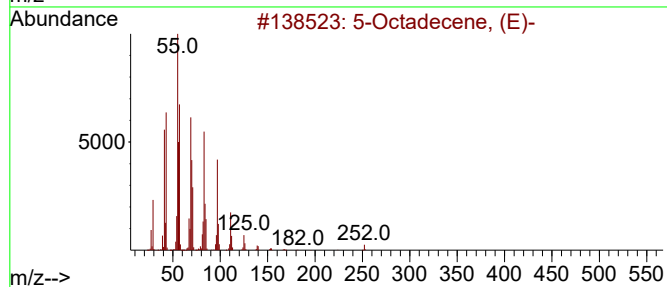
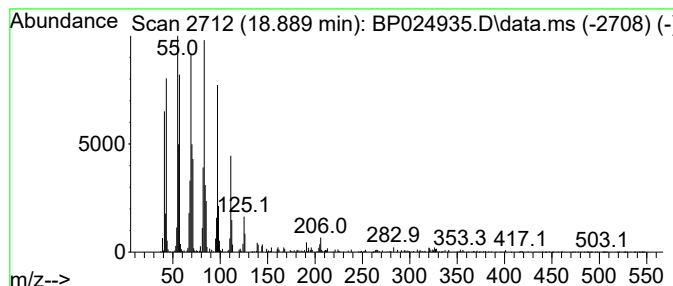
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.889	2.82 ng	392144	Phenanthrene-d10	17.054

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-		252	C18H36	007206-21-5	99
2	1-Heptadecene		238	C17H34	006765-39-5	97
3	1-Heneicosyl formate		340	C22H44O2	077899-03-7	96
4	1-Docosene		308	C22H44	001599-67-3	95
5	1-Hexadecanol		242	C16H34O	036653-82-4	94



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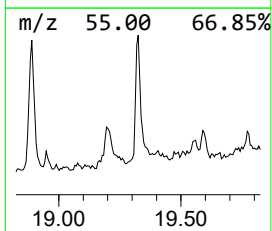
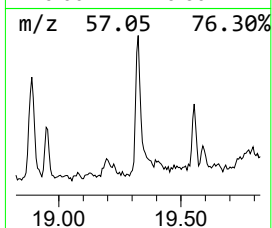
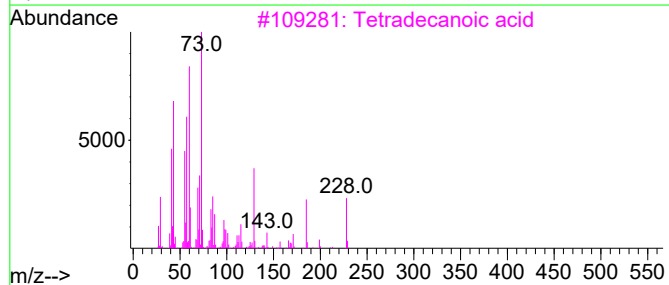
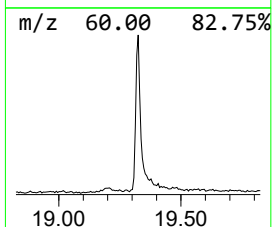
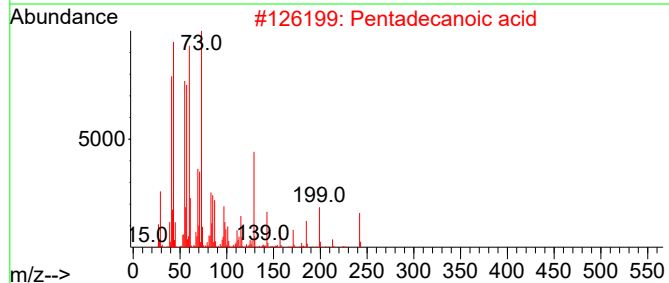
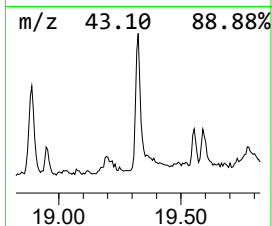
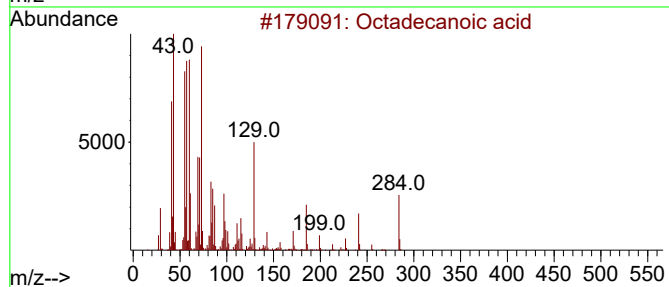
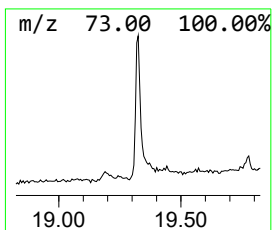
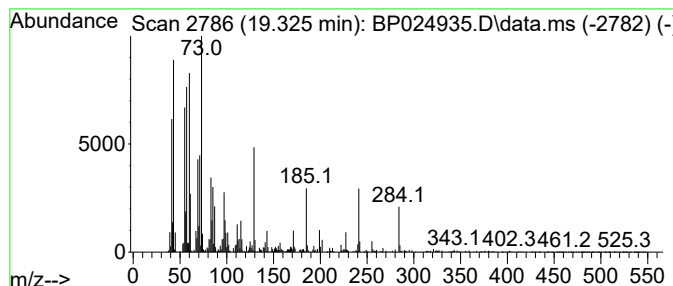
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.325	3.54 ng	646711	Chrysene-d12	21.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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TP-3

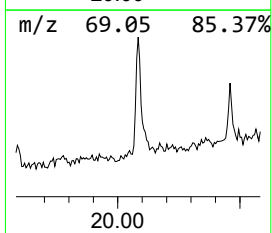
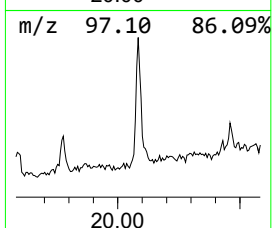
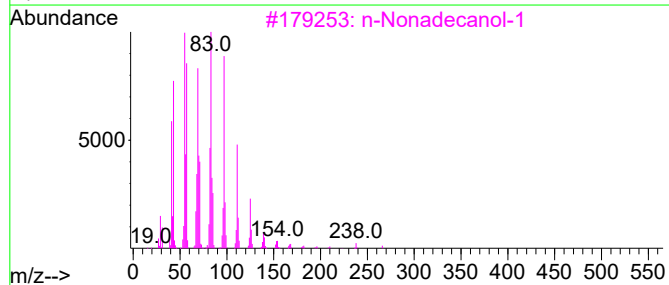
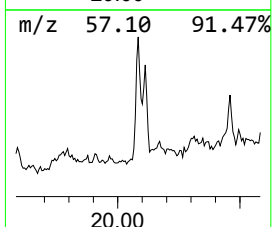
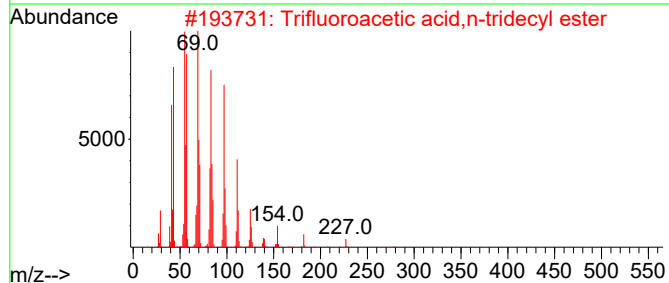
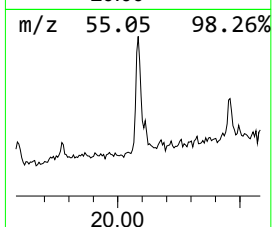
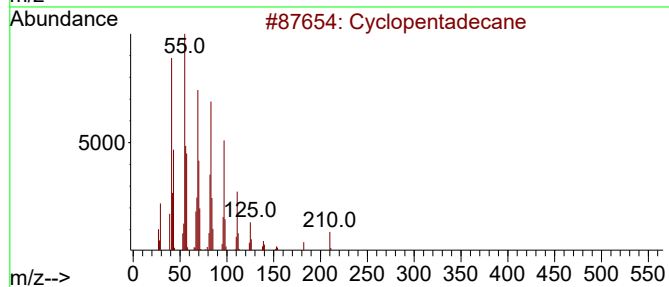
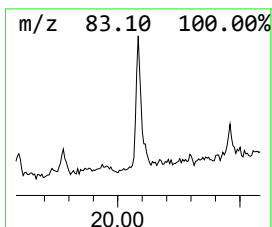
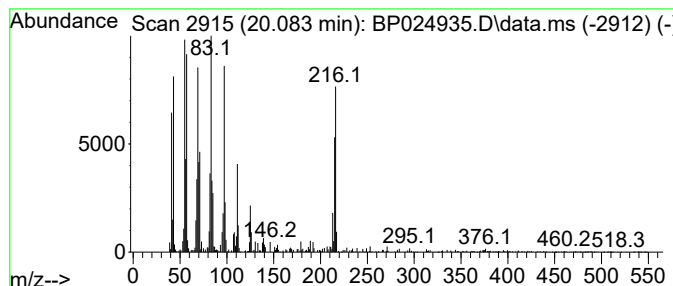
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.083	2.01 ng	367665	Chrysene-d12	21.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	89
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	89
4			1-Heneicosanol	312	C21H44O	015594-90-8	86
5			1-Nonadecene	266	C19H38	018435-45-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061225\
Data File : BP024935.D
Acq On : 12 Jun 2025 18:37
Operator : RC/JU
Sample : Q2297-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

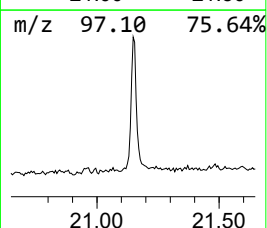
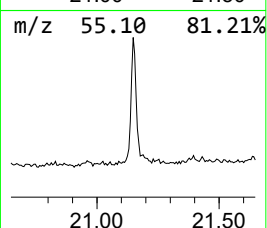
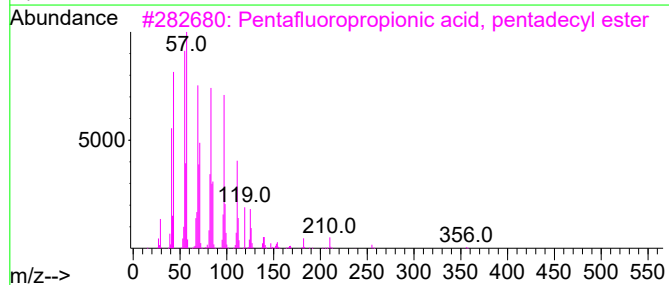
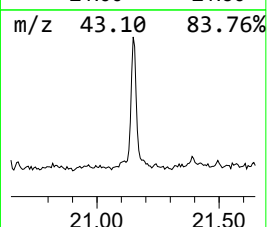
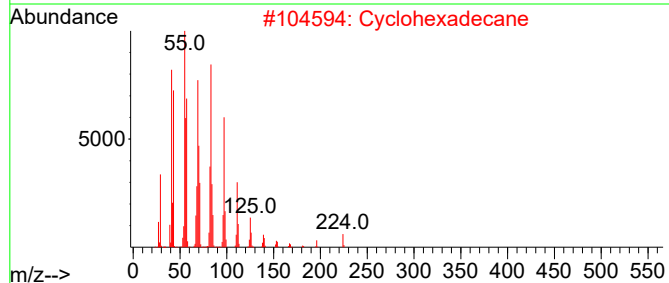
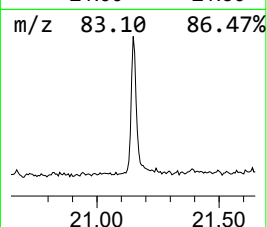
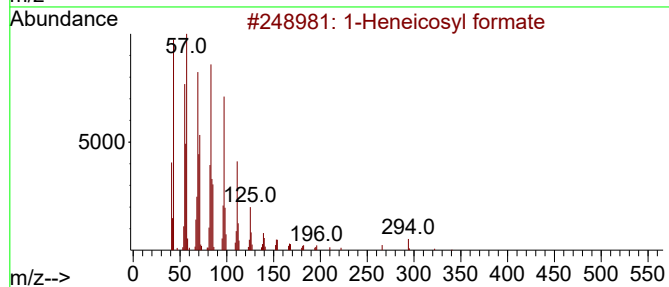
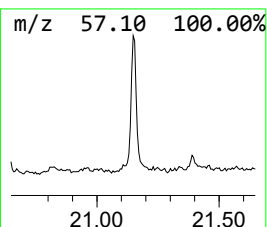
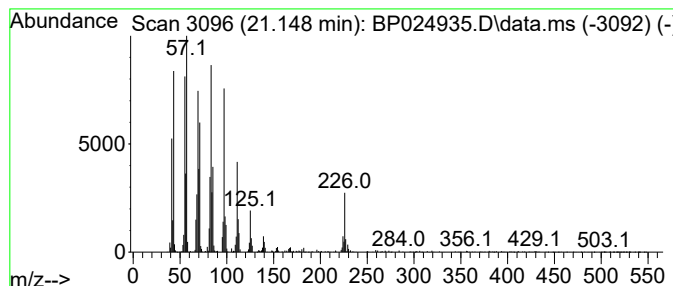
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.148	6.58 ng	1202270	Chrysene-d12	21.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			Cyclohexadecane	224	C16H32	000295-65-8	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061225\
Data File : BP024935.D
Acq On : 12 Jun 2025 18:37
Operator : RC/JU
Sample : Q2297-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

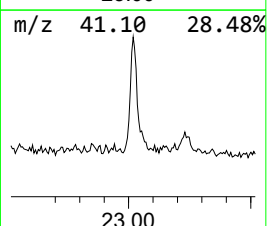
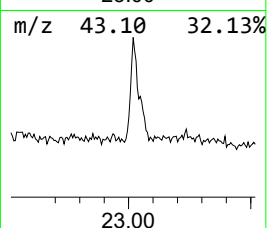
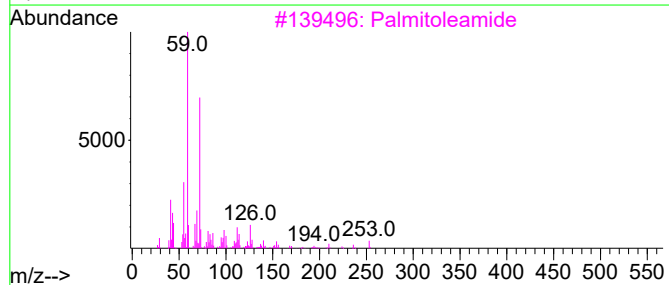
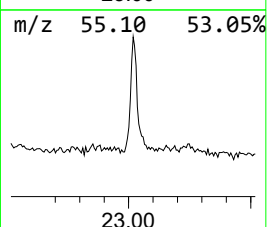
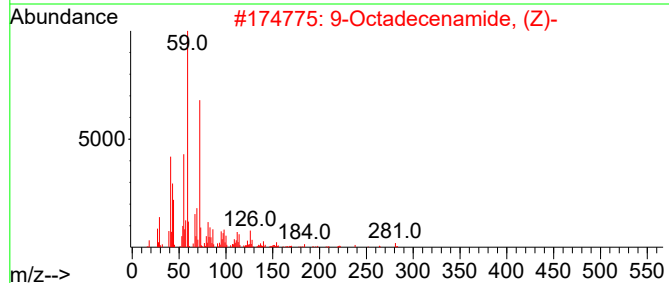
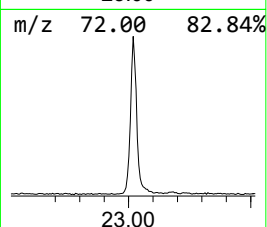
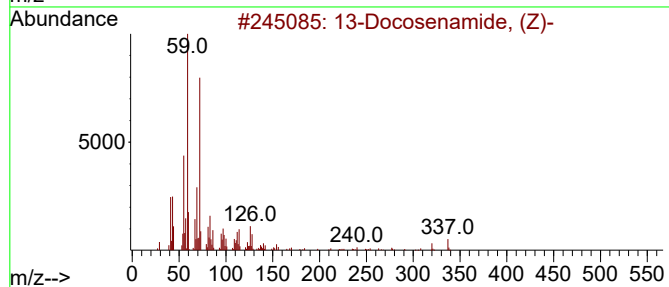
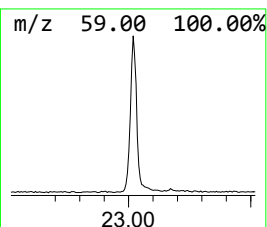
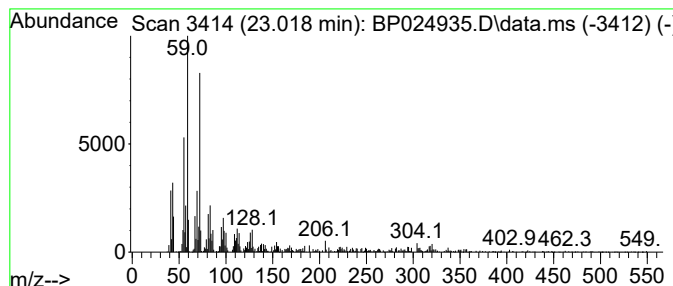
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.019	5.91 ng	1079860	Chrysene-d12	21.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
3			Palmitoleamide	253	C16H31NO	106010-22-4	74
4			Octadecanamide	283	C18H37NO	000124-26-5	50
5			9-Octadecenamide	281	C18H35NO	003322-62-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061225\
Data File : BP024935.D
Acq On : 12 Jun 2025 18:37
Operator : RC/JU
Sample : Q2297-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060625.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
2-Pentanone, 4-...	4.772	5.7	ng	386189	1	7.608	1349630	20.0
Benzophenone	15.642	12.2	ng	1452180	3	14.248	2388170	20.0
n-Hexadecanoic ...	17.995	12.3	ng	1715190	4	17.054	2781520	20.0
5-Octadecene, (E)-	18.889	2.8	ng	392144	4	17.054	2781520	20.0
Octadecanoic acid	19.325	3.5	ng	646711	5	21.483	3655610	20.0
Cyclopentadecane	20.083	2.0	ng	367665	5	21.483	3655610	20.0
1-Heneicosyl fo...	21.148	6.6	ng	1202270	5	21.483	3655610	20.0
13-Docosenamide...	23.019	5.9	ng	1079860	5	21.483	3655610	20.0