

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
 Data File : BP025388.D
 Acq On : 13 Aug 2025 17:32
 Operator : CG/JU
 Sample : Q2820-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 518R-S

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-BP080525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025388.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.967	3	5	14	rVB2	141086	233929	4.18%	0.488%
2	3.049	14	19	35	rVB	730957	1118767	20.00%	2.336%
3	4.955	336	343	348	rBV	209990	302673	5.41%	0.632%
4	5.413	414	421	433	rBV	2200748	3258977	58.25%	6.805%
5	6.108	533	539	552	rBV7	27227	70825	1.27%	0.148%
6	6.313	565	574	582	rBV7	24323	68293	1.22%	0.143%
7	6.466	591	600	603	rBV5	40400	84932	1.52%	0.177%
8	6.972	679	686	694	rBV	2078915	3256162	58.20%	6.799%
9	7.796	819	826	834	rVB	765981	1241812	22.19%	2.593%
10	8.096	869	877	884	rVB4	28833	62652	1.12%	0.131%
11	8.937	1004	1020	1028	rBV	1312445	2307940	41.25%	4.819%
12	10.572	1288	1298	1305	rBV	971283	1728935	30.90%	3.610%
13	13.031	1708	1716	1729	rBV	3011523	4729823	84.53%	9.876%
14	14.419	1945	1952	1959	rBV	1394593	2231130	39.88%	4.659%
15	15.795	2180	2186	2196	rVB	304399	480812	8.59%	1.004%
16	15.931	2201	2209	2218	rBV	2387354	3718624	66.46%	7.765%
17	16.372	2280	2284	2289	rVB	103161	143296	2.56%	0.299%
18	17.125	2408	2412	2415	rBV2	101413	139059	2.49%	0.290%
19	17.219	2420	2428	2433	rVV	1678557	2579737	46.11%	5.387%
20	17.260	2433	2435	2439	rVB	115935	129902	2.32%	0.271%
21	17.354	2448	2451	2456	rVB	62618	88870	1.59%	0.186%
22	18.042	2562	2568	2574	rBV3	76650	169698	3.03%	0.354%
23	18.095	2574	2577	2580	rBV3	52083	73416	1.31%	0.153%
24	18.166	2584	2589	2599	rBV	1298870	2015596	36.02%	4.209%
25	18.330	2612	2617	2620	rBV2	57951	98704	1.76%	0.206%
26	18.472	2638	2641	2650	rVB3	81723	133576	2.39%	0.279%
27	19.077	2735	2744	2749	rBV5	44320	134368	2.40%	0.281%
28	19.224	2766	2769	2779	rVB	48919	78423	1.40%	0.164%
29	19.354	2786	2791	2797	rBV	785127	1109344	19.83%	2.316%
30	19.495	2811	2815	2828	rBV2	341090	639734	11.43%	1.336%
31	19.695	2845	2849	2850	rBV	101601	120842	2.16%	0.252%
32	19.730	2850	2855	2860	rVB	770193	1027961	18.37%	2.146%
33	19.942	2885	2891	2902	rVB	4070622	5595208	100.00%	11.683%
34	20.407	2966	2970	2973	rBV2	72432	115205	2.06%	0.241%
35	21.342	3126	3129	3143	rVB4	543720	925478	16.54%	1.932%
36	21.677	3177	3186	3191	rBV3	1683251	3569657	63.80%	7.454%

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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-BP080525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.718	3191	3193	3204	rVB	373242	579246	10.35%	1.209%
38	23.989	3573	3579	3587	rBV	255673	725722	12.97%	1.515%
39	25.071	3756	3763	3773	rBV	960335	2802989	50.10%	5.853%

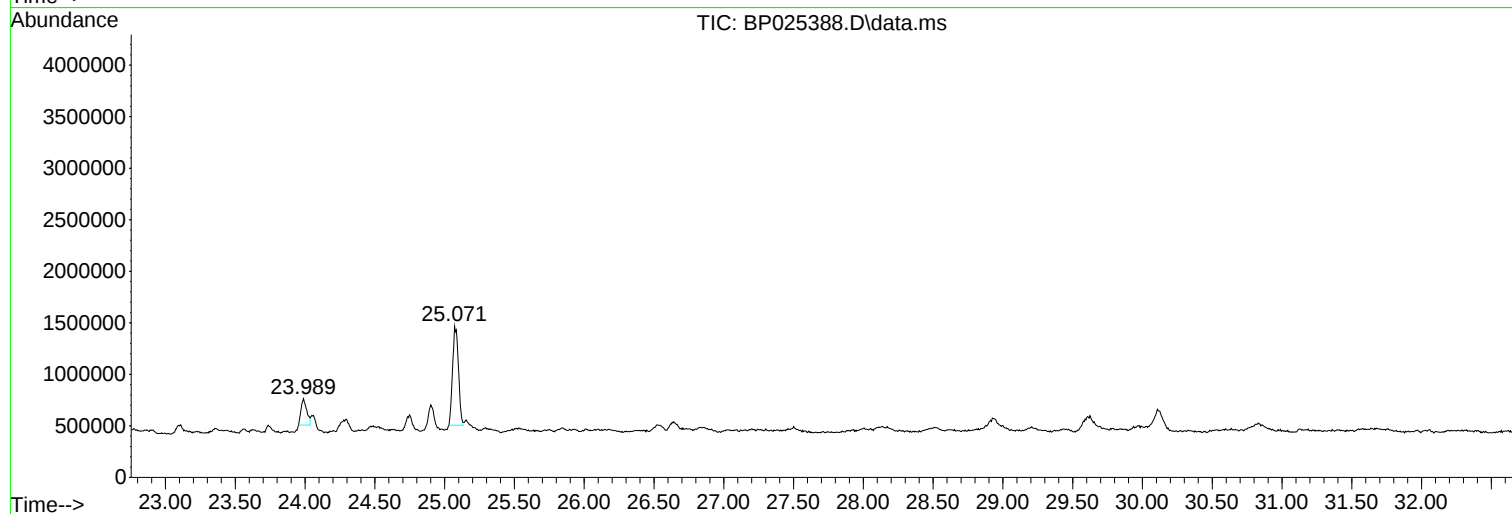
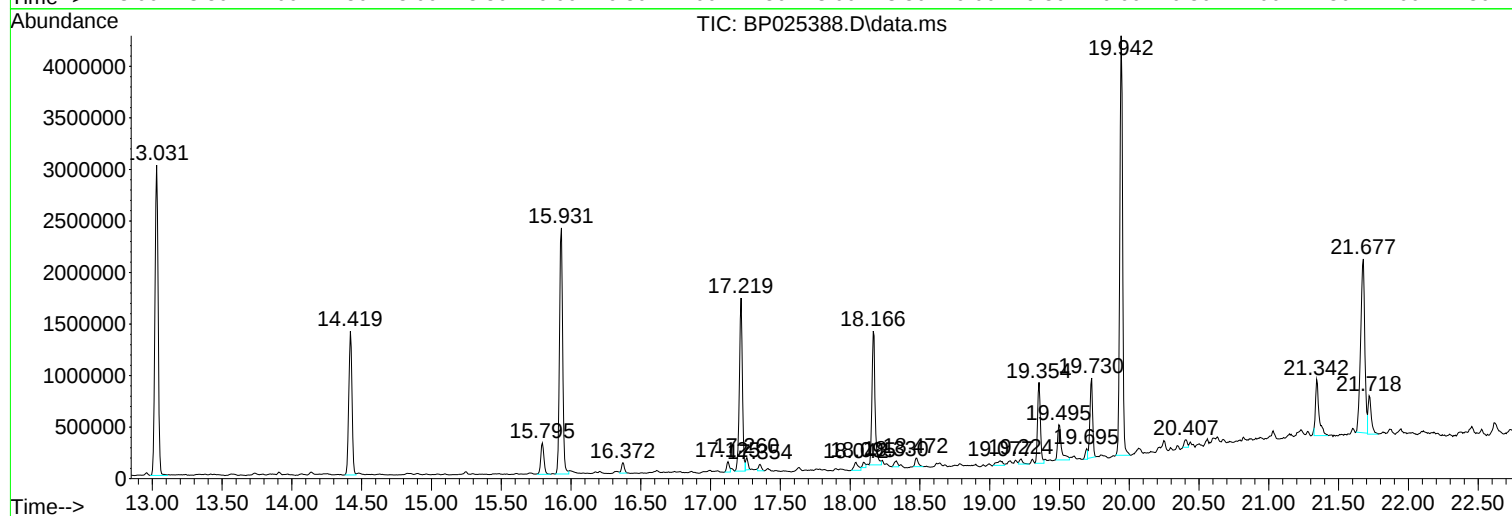
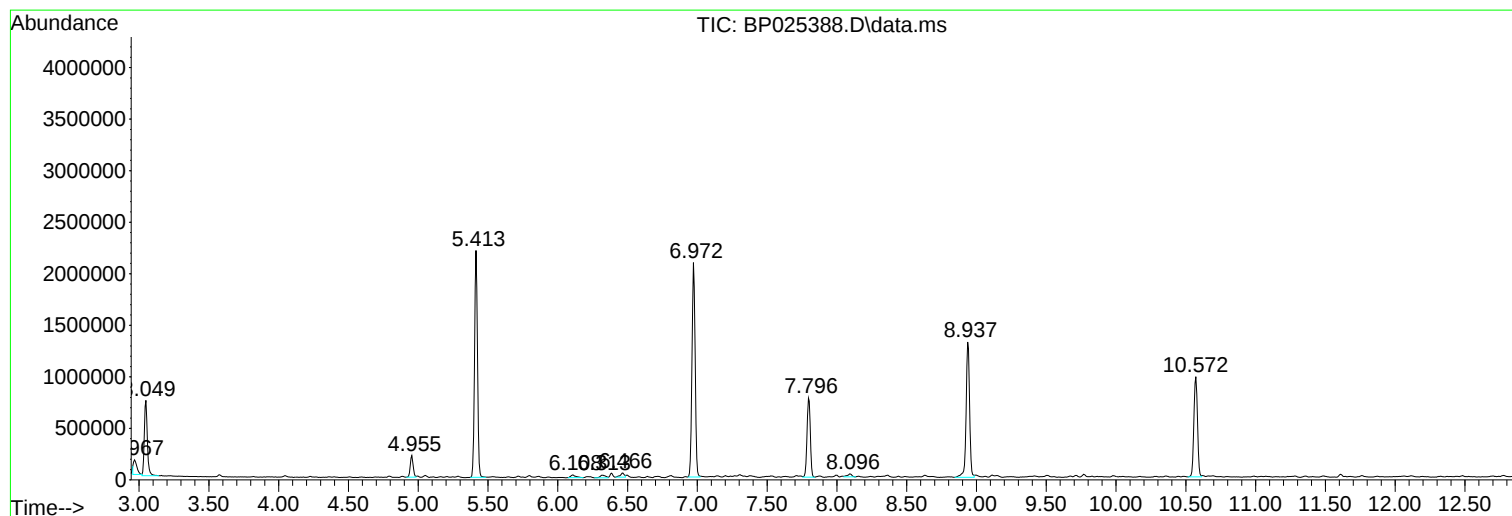
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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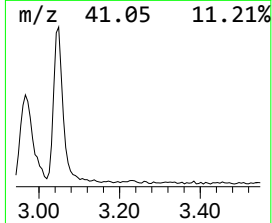
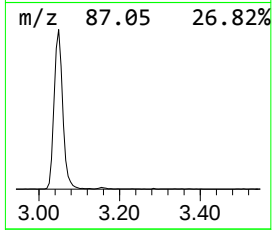
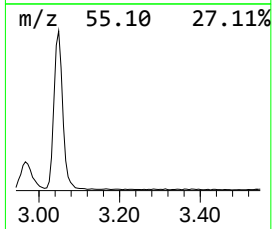
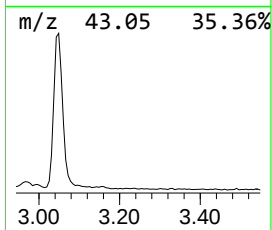
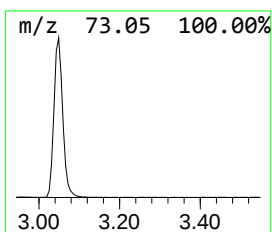
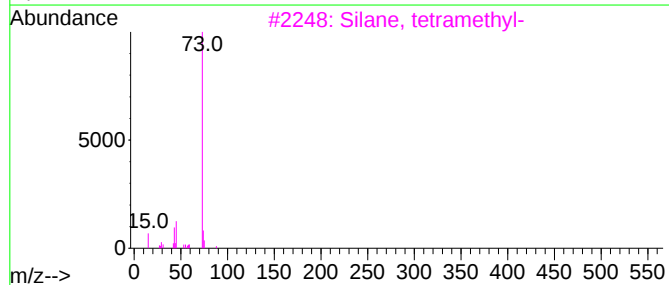
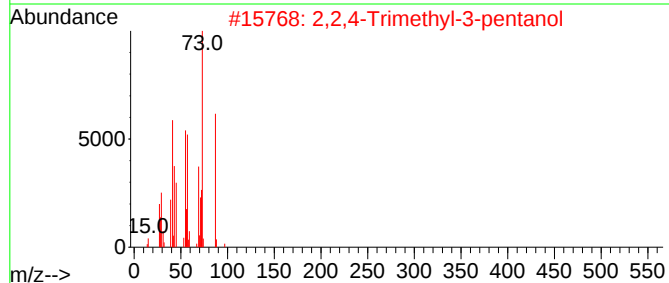
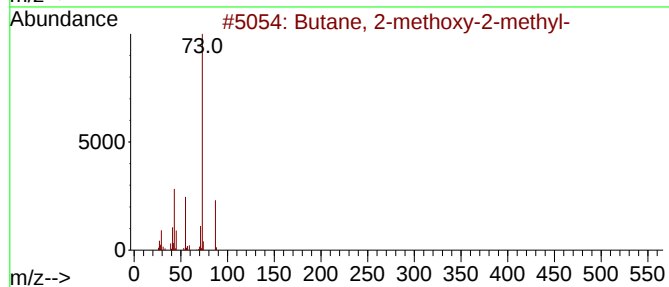
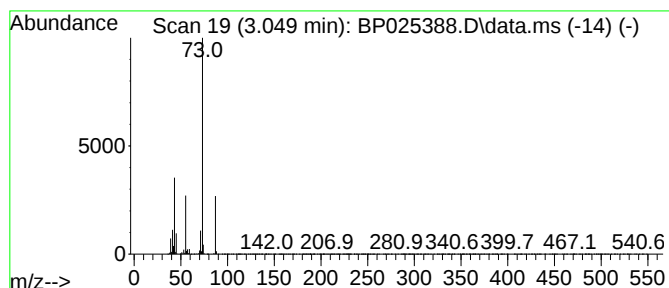
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.049	18.02 ng	1118770	1,4-Dichlorobenzene-d4	7.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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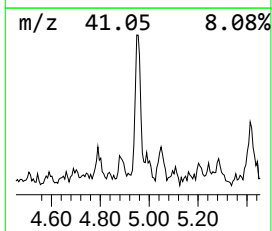
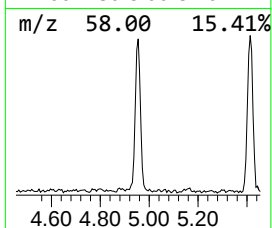
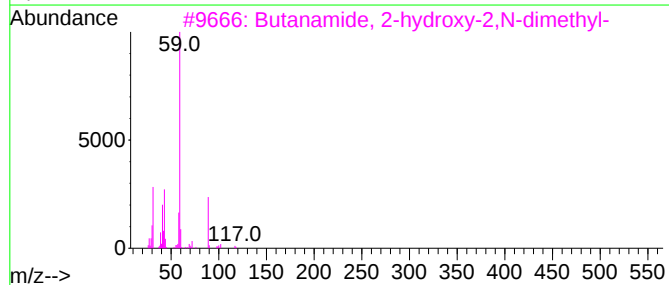
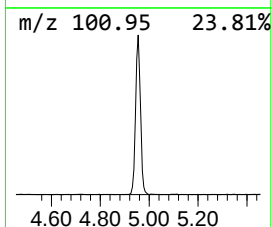
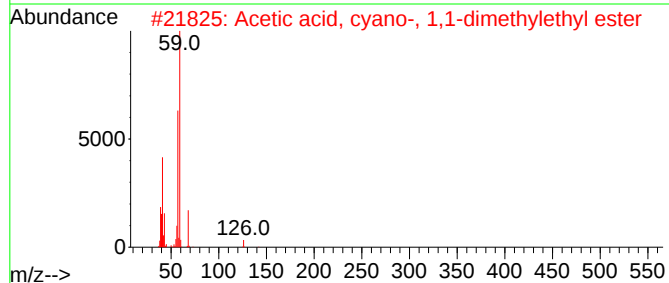
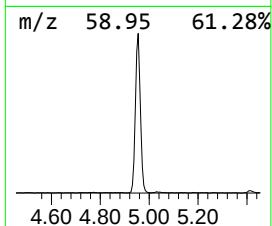
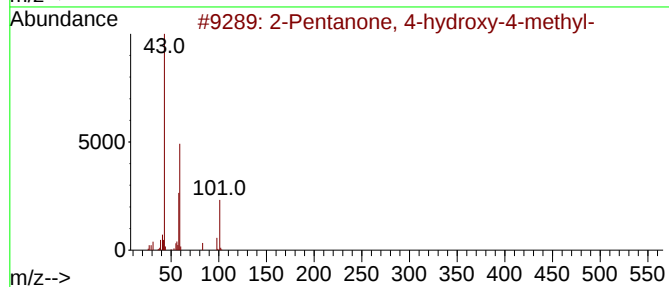
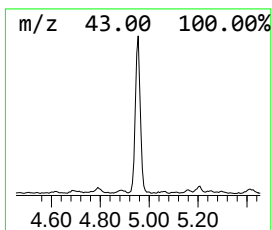
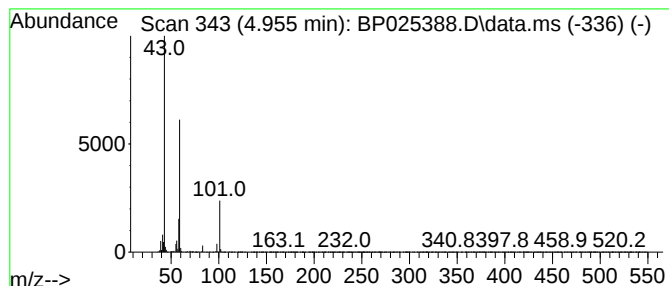
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.955	4.87 ng	302673	1,4-Dichlorobenzene-d4	7.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	23
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17



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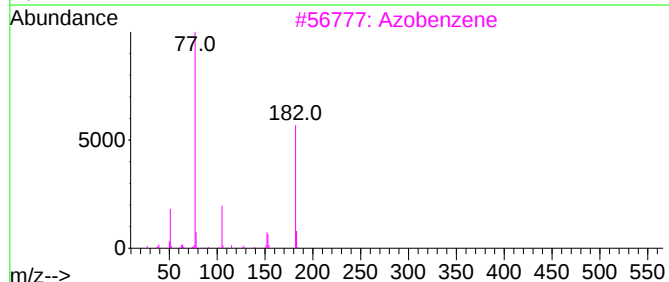
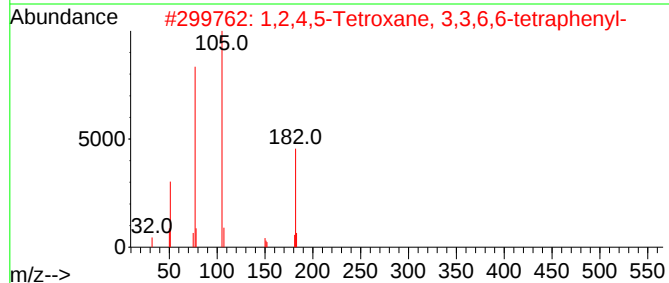
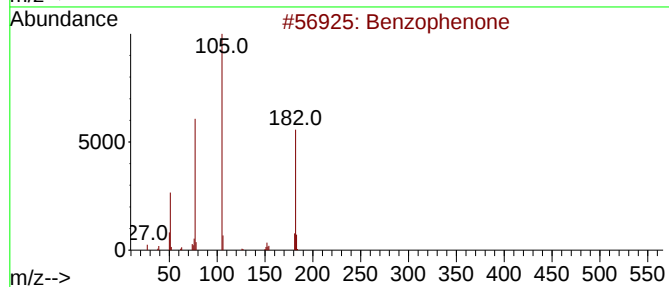
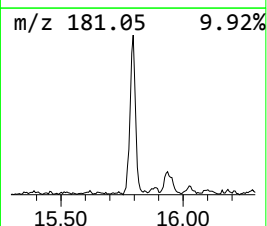
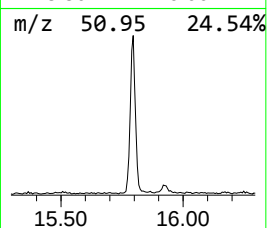
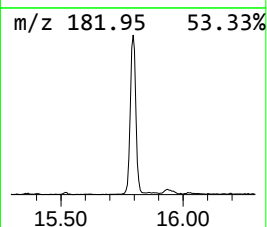
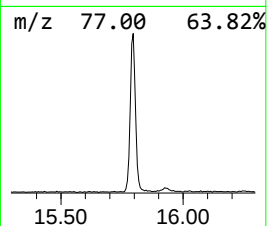
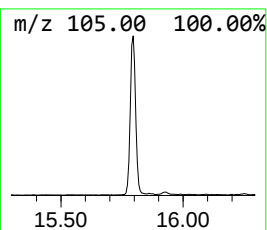
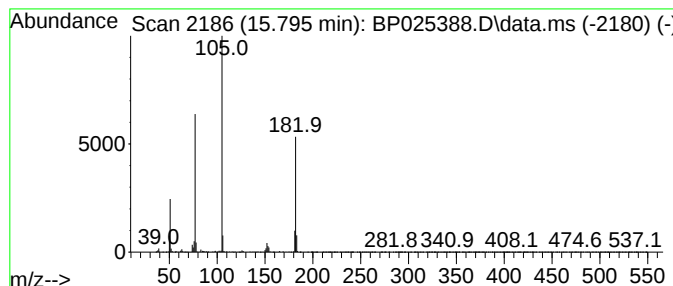
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.795	4.31 ng	480812	Acenaphthene-d10	14.419

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	78
3			Azobenzene	182	C12H10N2	000103-33-3	59
4			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
5			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50



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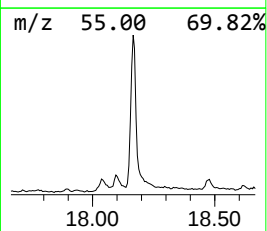
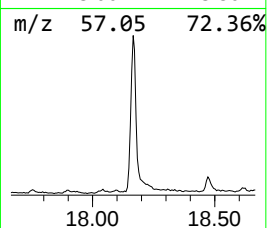
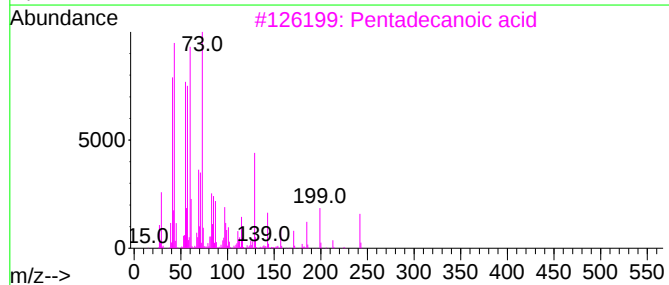
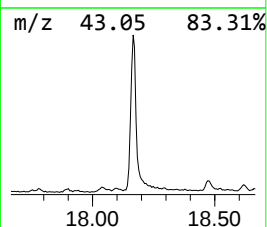
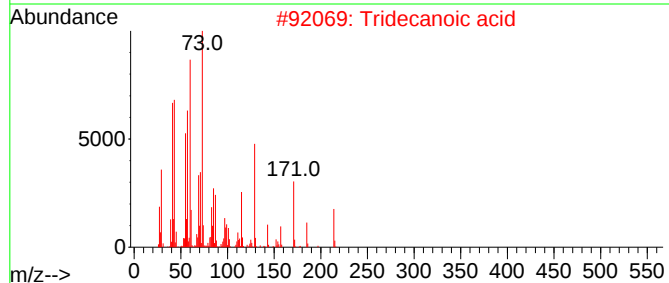
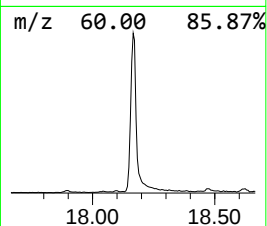
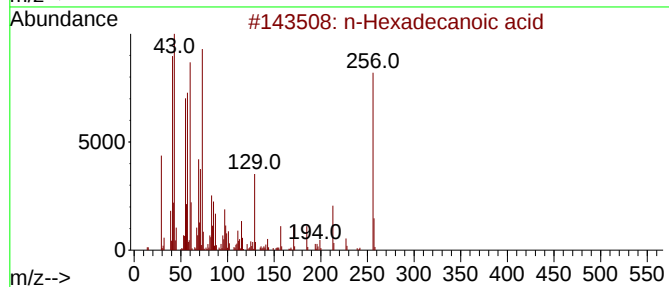
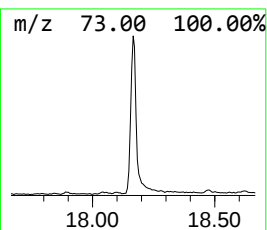
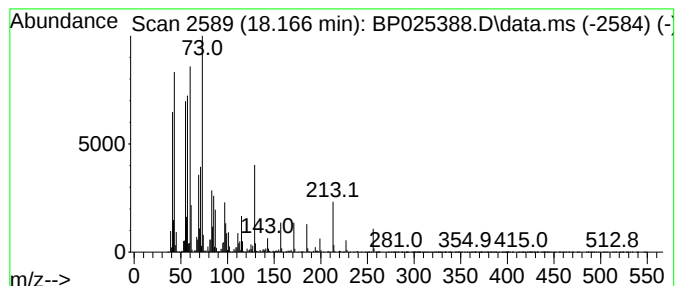
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.166	15.63 ng	2015600	Phenanthrene-d10	17.219	
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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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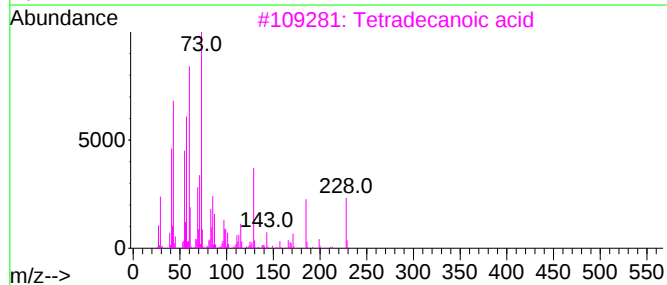
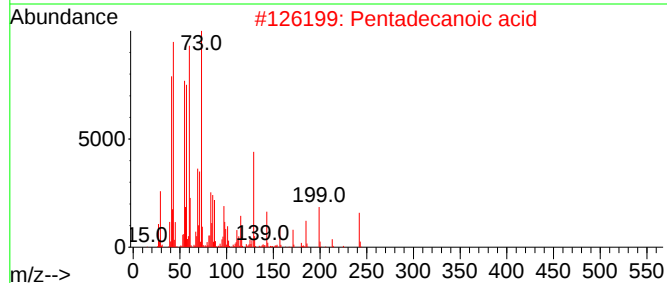
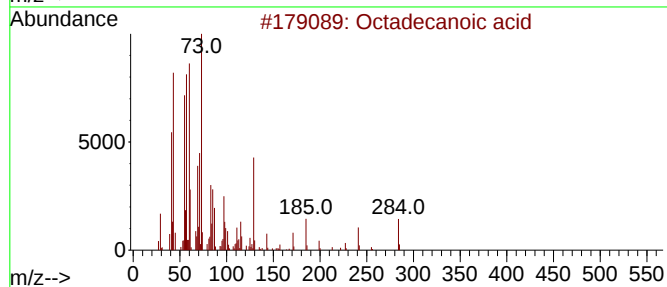
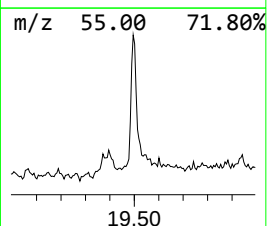
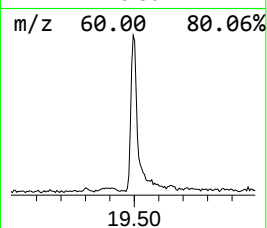
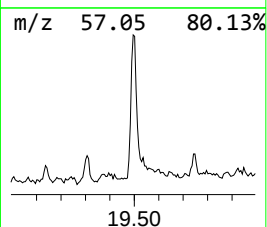
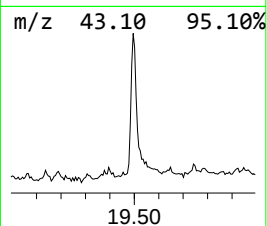
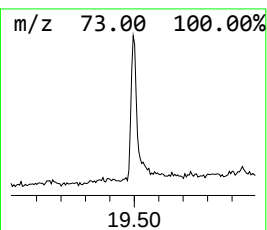
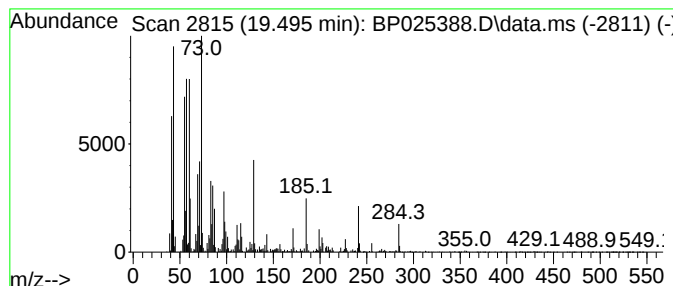
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.495	3.58 ng	639734	Chrysene-d12	21.677

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	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025388.D
Acq On : 13 Aug 2025 17:32
Operator : CG/JU
Sample : Q2820-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
518R-S

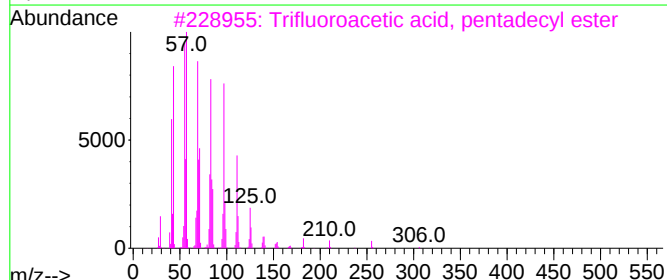
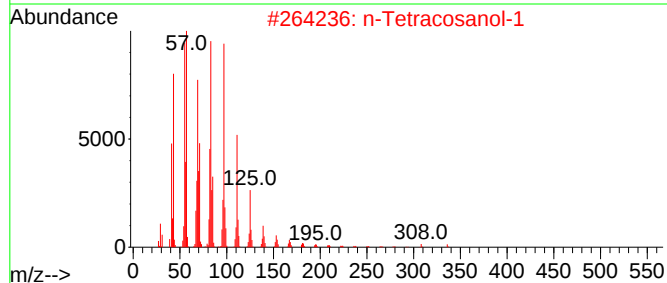
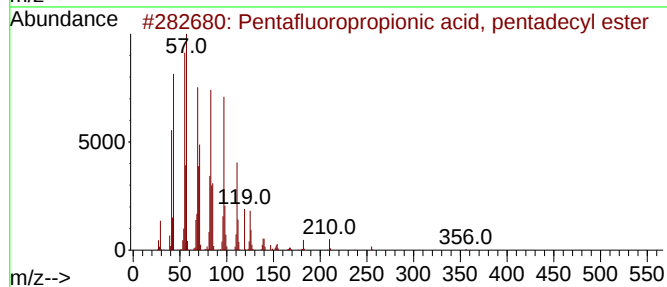
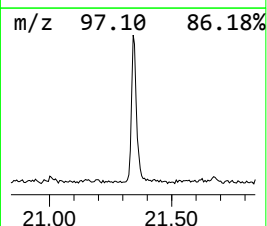
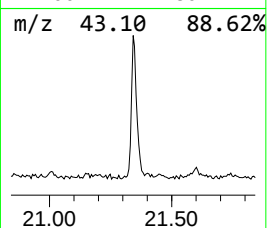
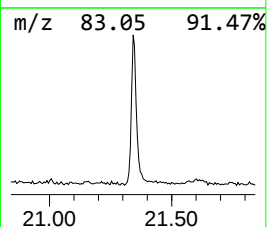
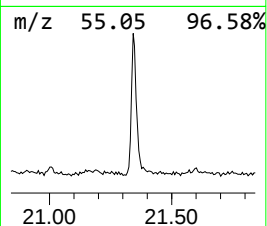
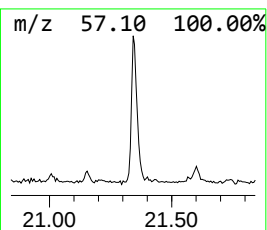
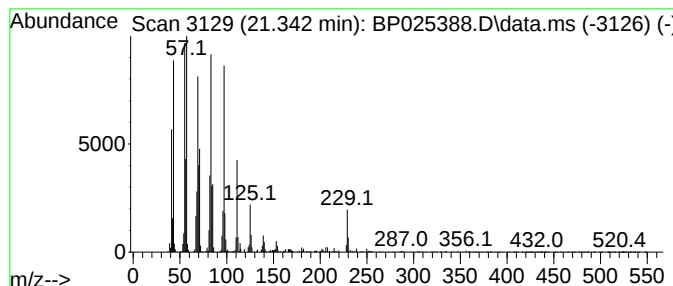
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.342	5.19 ng	925478	Chrysene-d12	21.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025388.D
Acq On : 13 Aug 2025 17:32
Operator : CG/JU
Sample : Q2820-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
518R-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.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
Butane, 2-metho...	3.049	18.0	ng	1118770	1	7.796	1241810	20.0
2-Pentanone, 4-...	4.955	4.9	ng	302673	1	7.796	1241810	20.0
Benzophenone	15.795	4.3	ng	480812	3	14.419	2231130	20.0
n-Hexadecanoic ...	18.166	15.6	ng	2015600	4	17.219	2579740	20.0
Octadecanoic acid	19.495	3.6	ng	639734	5	21.677	3569660	20.0
Pentafluoroprop...	21.342	5.2	ng	925478	5	21.677	3569660	20.0