

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032522\
 Data File : BP009557.D
 Acq On : 25 Mar 2022 17:52
 Operator : CG/JU
 Sample : N2109-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-1

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-BP031722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	3	5	20	rVB	475866	701412	5.95%	0.721%
2	5.375	399	406	426	rBV	3437926	6133117	52.03%	6.305%
3	6.957	666	675	699	rBV	3325827	6438155	54.62%	6.619%
4	7.769	806	813	823	rBV	788974	1427392	12.11%	1.468%
5	8.922	1001	1009	1022	rBV	2112857	4051703	34.37%	4.166%
6	10.557	1277	1287	1304	rBV	978073	2039965	17.31%	2.097%
7	13.034	1700	1708	1732	rBV	5527100	8922565	75.70%	9.173%
8	14.133	1882	1895	1912	rBV	279706	545095	4.62%	0.560%
9	14.410	1935	1942	1951	rBV	1581570	2678723	22.73%	2.754%
10	15.910	2190	2197	2222	rBV	4161815	7272515	61.70%	7.477%
11	16.151	2234	2238	2252	rVB2	76985	153840	1.31%	0.158%
12	17.174	2406	2412	2417	rBV	2006866	3174874	26.94%	3.264%
13	17.222	2417	2420	2428	rVV	471186	693931	5.89%	0.713%
14	17.316	2431	2436	2442	rVB	177532	306238	2.60%	0.315%
15	18.051	2557	2561	2564	rBV	113564	161299	1.37%	0.166%
16	18.098	2564	2569	2576	rVB2	199749	397125	3.37%	0.408%
17	18.239	2588	2593	2597	rBV3	169388	313974	2.66%	0.323%
18	18.274	2597	2599	2606	rVB	99863	137086	1.16%	0.141%
19	18.539	2640	2644	2648	rBV	103685	142518	1.21%	0.147%
20	18.945	2709	2713	2717	rBV	139385	210105	1.78%	0.216%
21	18.998	2717	2722	2726	rVV4	65342	146383	1.24%	0.150%
22	19.086	2733	2737	2744	rBV4	85453	161229	1.37%	0.166%
23	19.204	2751	2757	2764	rBV	2036259	2958441	25.10%	3.042%
24	19.351	2778	2782	2786	rVB	186932	252095	2.14%	0.259%
25	19.557	2808	2817	2826	rBV	1862534	3166469	26.86%	3.255%
26	19.627	2827	2829	2836	rVB2	93379	146887	1.25%	0.151%
27	19.757	2844	2851	2864	rVB	9001097	11786801	100.00%	12.118%
28	19.874	2866	2871	2878	rBV3	189495	453784	3.85%	0.467%
29	20.010	2890	2894	2896	rBV3	160798	259379	2.20%	0.267%
30	20.039	2897	2899	2908	rVB2	329888	464044	3.94%	0.477%
31	20.145	2913	2917	2921	rVV	172019	220888	1.87%	0.227%
32	20.198	2922	2926	2930	rVB2	248156	364075	3.09%	0.374%
33	20.333	2946	2949	2953	rBV	134968	180866	1.53%	0.186%
34	20.380	2954	2957	2961	rVV	147564	186000	1.58%	0.191%
35	20.780	3022	3025	3031	rVB	211857	291559	2.47%	0.300%
36	20.945	3050	3053	3056	rVB2	169526	197547	1.68%	0.203%

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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-BP031722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.980	3056	3059	3062	rVB	202520	213542	1.81%	0.220%
38	21.039	3063	3069	3073	rBV4	265220	739056	6.27%	0.760%
39	21.292	3105	3112	3116	rBV2	3383872	6807811	57.76%	6.999%
40	21.327	3116	3118	3126	rVB	1564467	1886443	16.00%	1.939%
41	21.410	3127	3132	3145	rBV	5585703	8581197	72.80%	8.822%
42	22.962	3390	3396	3401	rBV	1532262	3681927	31.24%	3.785%
43	23.474	3478	3483	3492	rVB	879368	1787009	15.16%	1.837%
44	23.574	3495	3500	3510	rVB	1275551	2848451	24.17%	2.929%
45	23.680	3512	3518	3525	rBV2	1668991	3582761	30.40%	3.683%

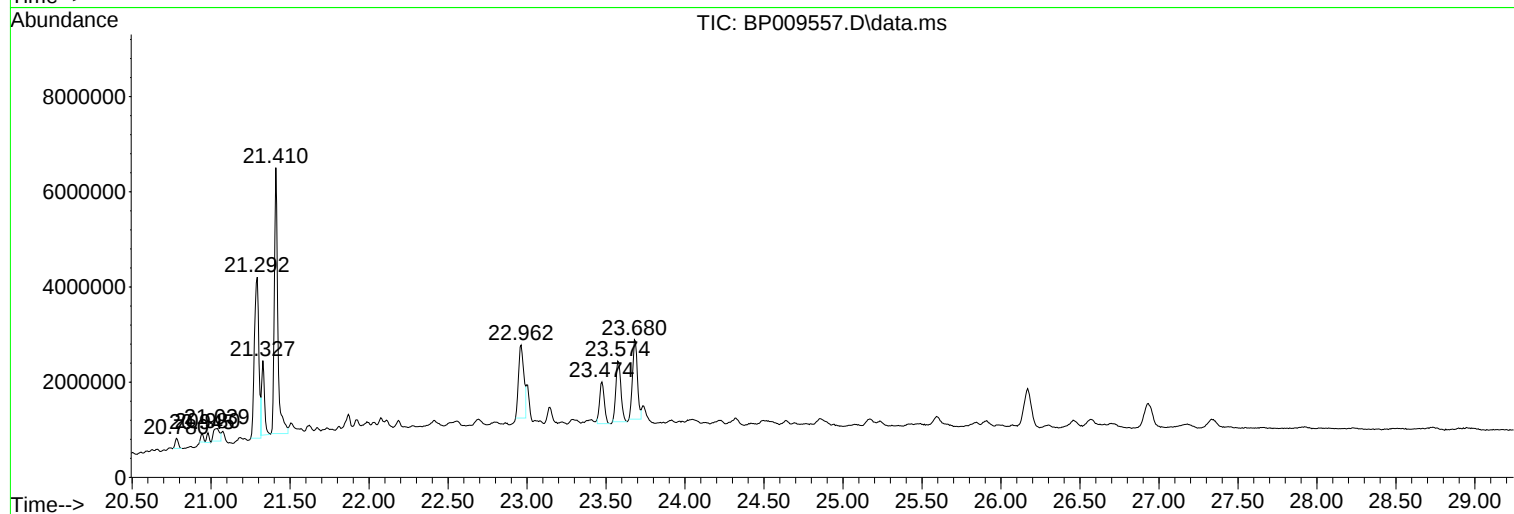
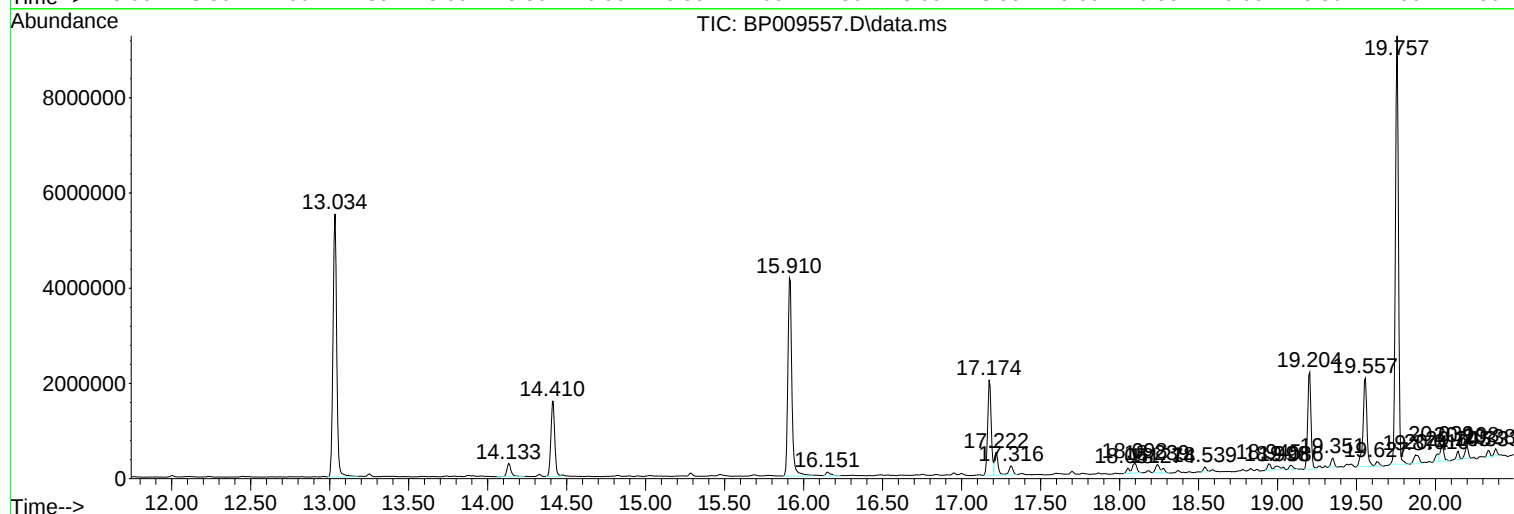
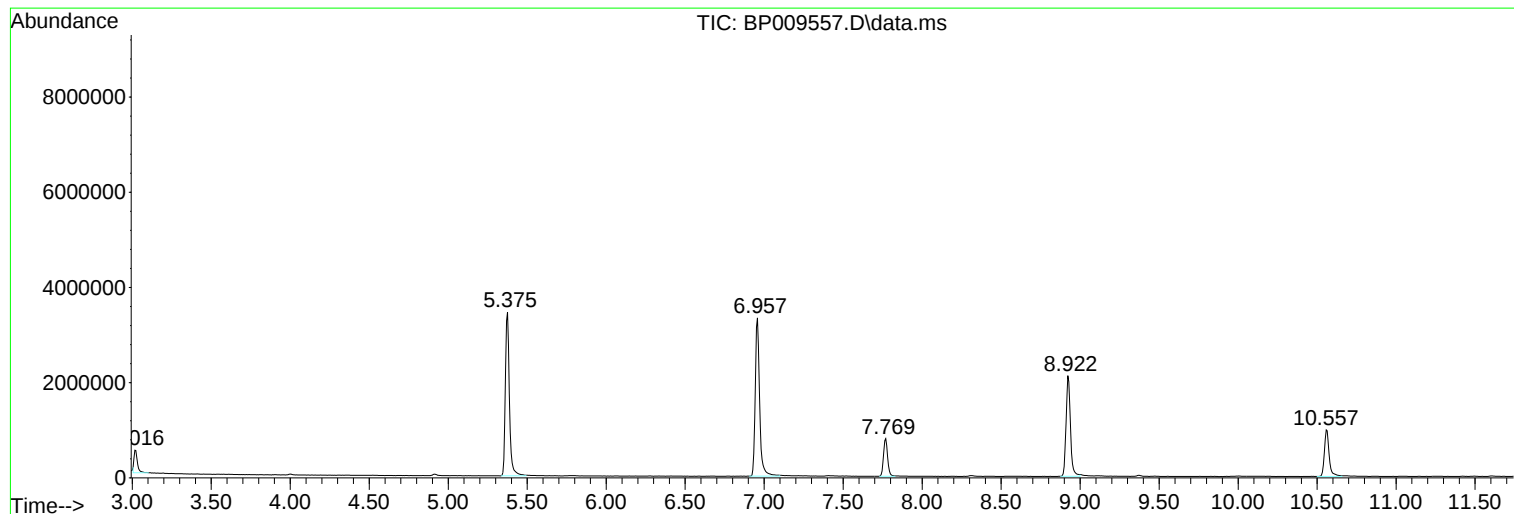
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
Sample : N2109-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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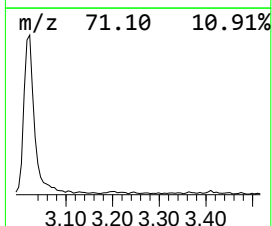
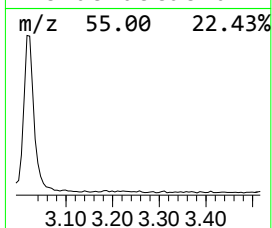
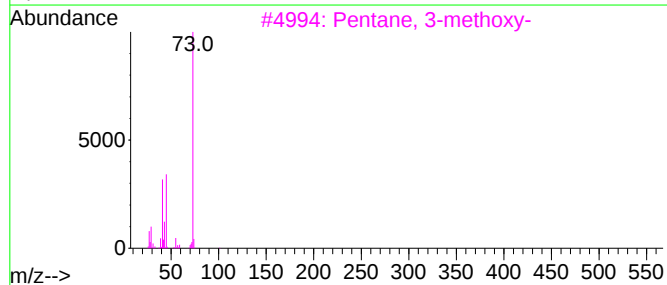
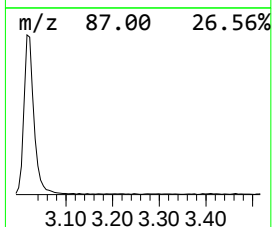
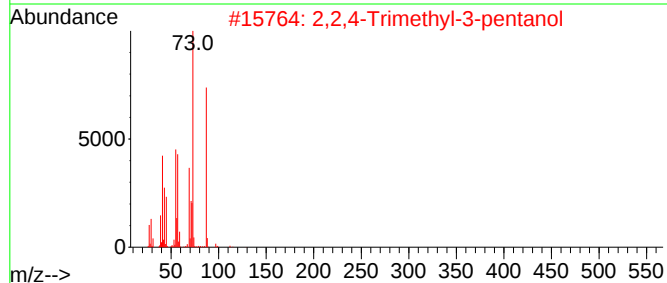
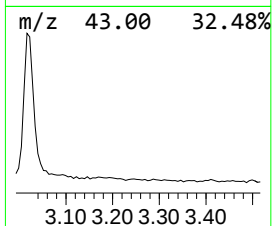
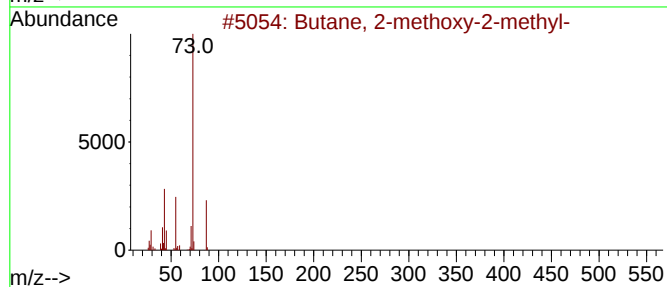
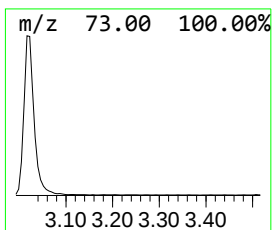
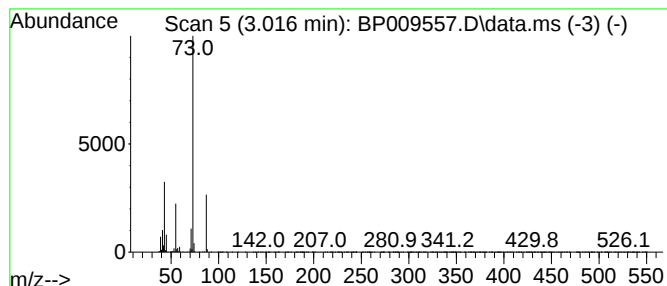
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.016	9.83 ng	701412	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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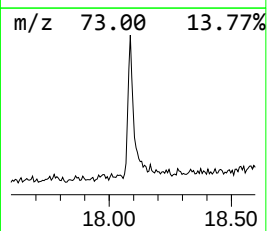
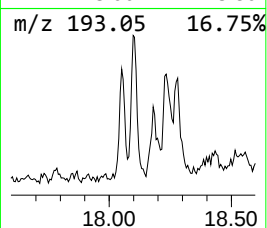
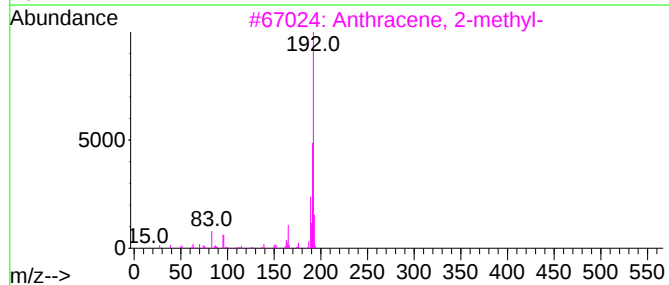
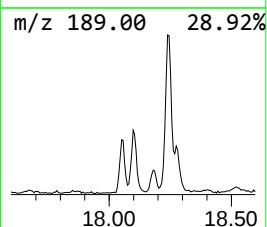
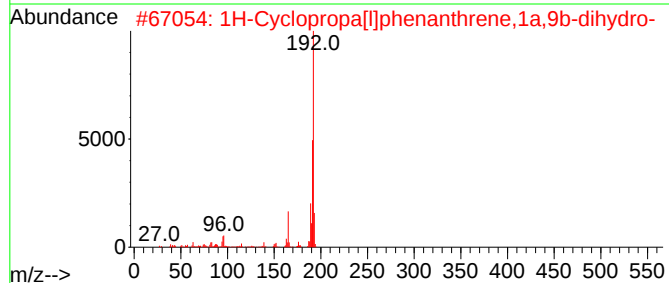
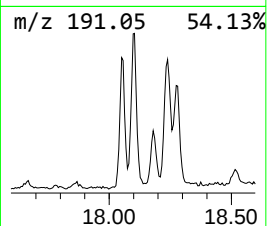
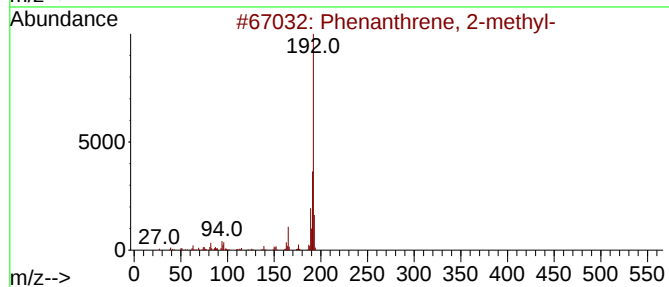
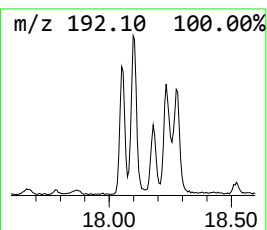
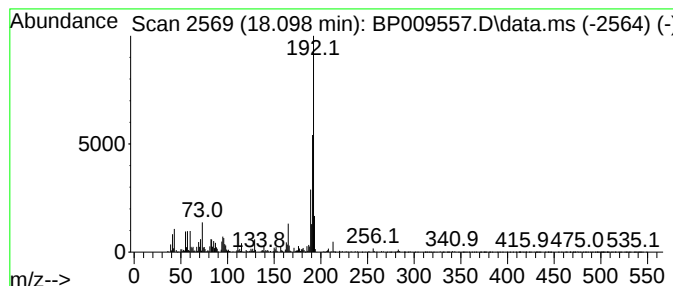
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	2.50 ng	397125	Phenanthrene-d10	17.174

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	97
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
5		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	95



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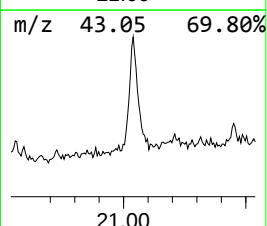
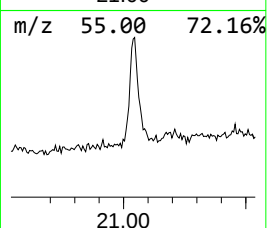
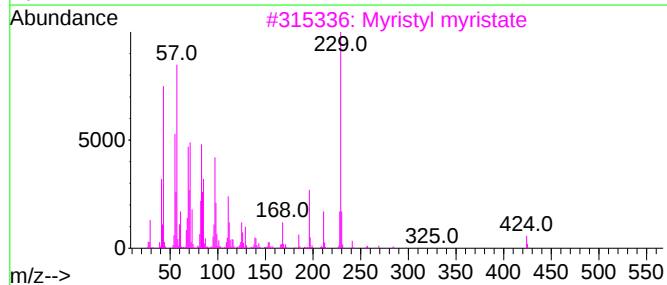
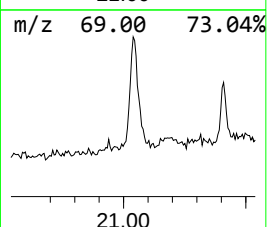
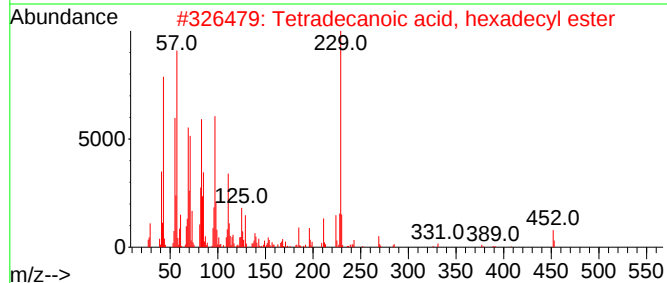
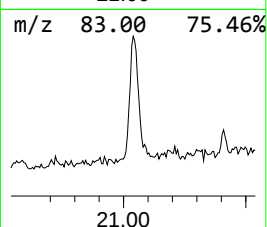
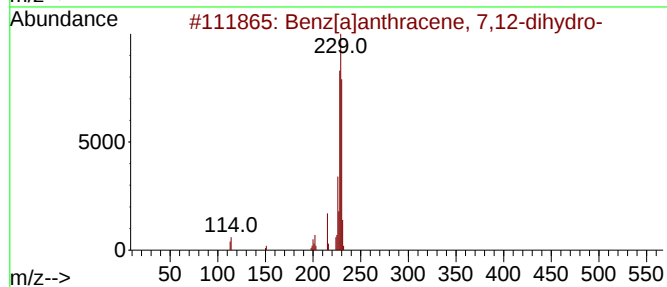
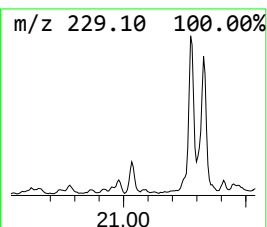
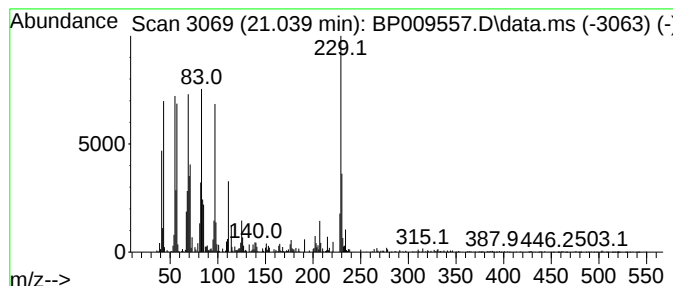
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown21.039 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.039	2.17 ng	739056	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[a]anthracene, 7,12-dihydro-	230	C18H14	016434-59-6	45
2			Tetradecanoic acid, hexadecyl ester	452	C30H60O2	002599-01-1	37
3			Myristyl myristate	424	C28H56O2	003234-85-3	32
4			Tetradecane, 1,1'-thiobis-	426	C28H58S	035599-83-8	32
5			Cyclohexane, (1-hexadecylheptade...	547	C39H78	055517-75-4	32



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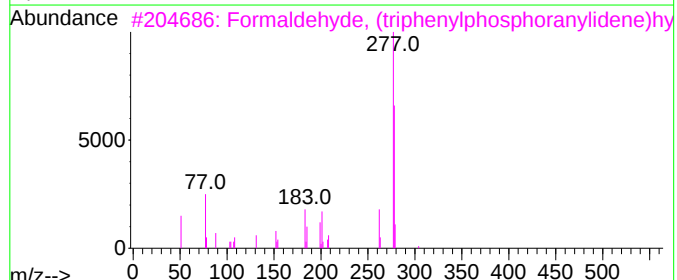
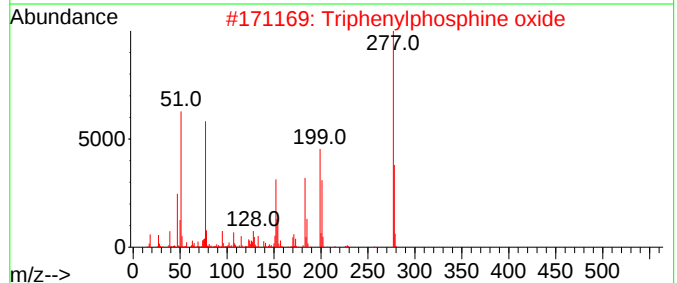
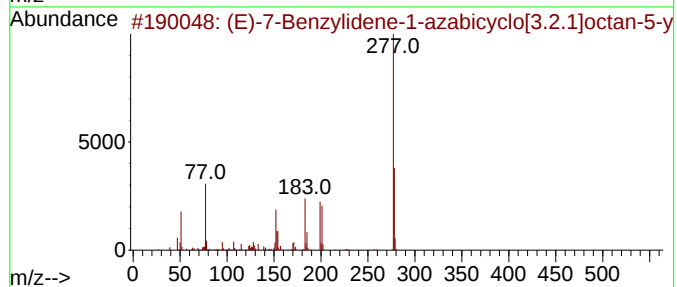
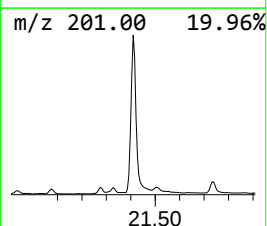
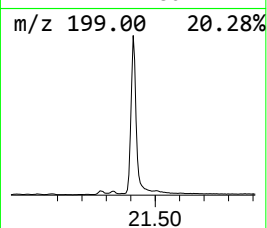
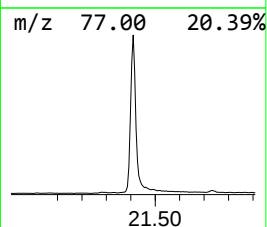
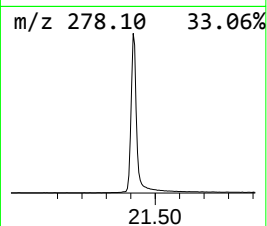
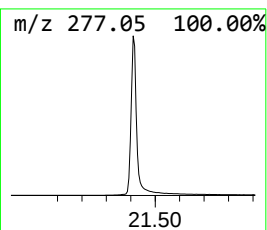
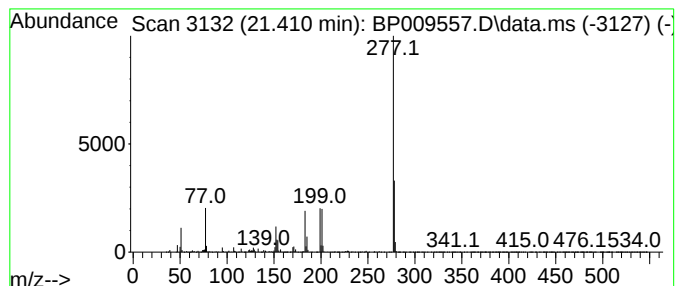
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	25.21 ng	8581200	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl	293	C15H19NO3S	1000483-83-4	91		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91		
3	Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	42		
4	Vanadium, cycloheptatrienyl-(pen...)	277	C17H22V	1000155-20-5	32		
5	Oxoprophines	277	C17H11NO3	1000128-51-1	9		



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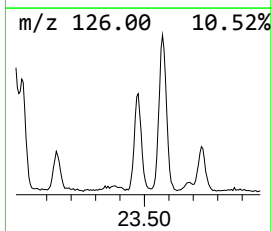
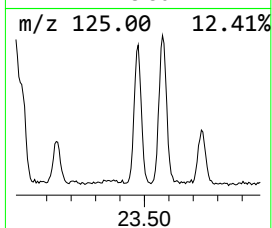
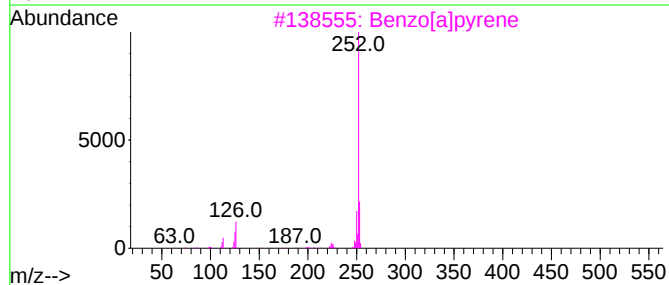
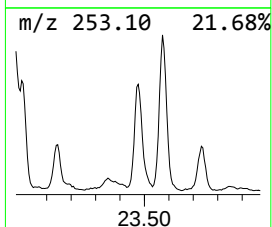
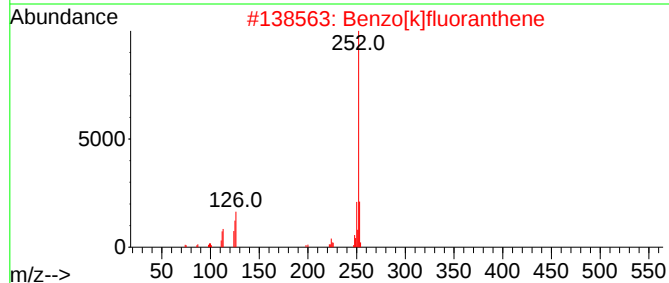
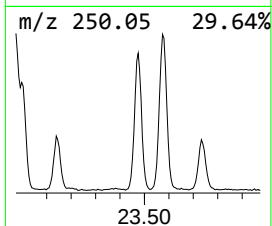
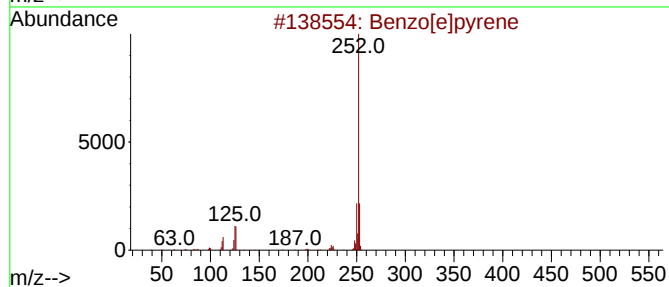
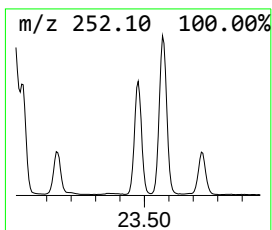
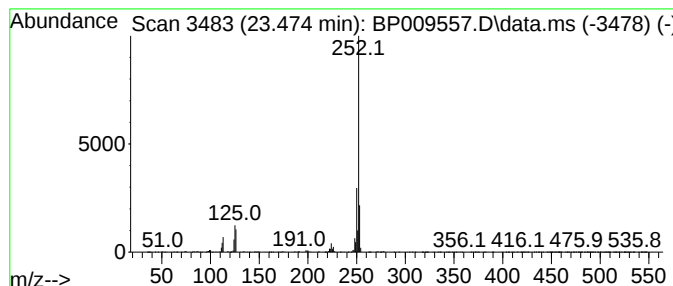
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.474	9.98 ng	1787010	Perylene-d12	23.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Benzo[a]pyrene	252	C20H12	000050-32-8	96
4			Perylene	252	C20H12	000198-55-0	96
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032522\
Data File : BP009557.D
Acq On : 25 Mar 2022 17:52
Operator : CG/JU
Sample : N2109-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.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...	3.016	9.8	ng	701412	1	7.769	1427390	20.0
Phenanthrene, 2...	18.098	2.5	ng	397125	4	17.174	3174870	20.0
unknown21.039	21.039	2.2	ng	739056	5	21.292	6807810	20.0
(E)-7-Benzylide...	21.410	25.2	ng	8581200	5	21.292	6807810	20.0
Benzo[e]pyrene	23.474	10.0	ng	1787010	6	23.680	3582760	20.0