

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
 Data File : BP021612.D
 Acq On : 22 Aug 2024 13:39
 Operator : RC/JU
 Sample : P3671-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-905-KJ-SO-0-0.5-081924-FD

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-BP081324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021612.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	14	rBV	3884017	5180505	48.24%	4.474%
2	3.552	91	96	105	rVB	226659	311672	2.90%	0.269%
3	4.940	326	332	339	rVB	265261	374295	3.49%	0.323%
4	5.399	404	410	418	rBV	4300709	6532859	60.83%	5.642%
5	6.969	669	677	686	rBV	4307095	7087550	65.99%	6.121%
6	7.799	810	818	825	rBV	1378546	2117909	19.72%	1.829%
7	8.946	1004	1013	1024	rBV	2478106	4261453	39.68%	3.680%
8	9.510	1102	1109	1117	rBV	100005	159624	1.49%	0.138%
9	10.587	1284	1292	1307	rBV	1729100	2977683	27.73%	2.572%
10	11.334	1410	1419	1431	rBV2	173641	415267	3.87%	0.359%
11	13.063	1704	1713	1724	rBV	5010370	6744853	62.80%	5.825%
12	14.451	1940	1949	1956	rBV	2472015	4002980	37.27%	3.457%
13	14.516	1956	1960	1966	rVB	98827	145406	1.35%	0.126%
14	14.675	1978	1987	1999	rVB4	85214	231062	2.15%	0.200%
15	15.963	2199	2206	2215	rBV	5238525	7166294	66.73%	6.189%
16	17.245	2418	2424	2429	rBV	3221332	4949485	46.08%	4.274%
17	17.292	2429	2432	2439	rVV	962567	1413356	13.16%	1.221%
18	17.392	2441	2449	2455	rVB	233223	425797	3.96%	0.368%
19	17.669	2487	2496	2507	rVB	130314	249749	2.33%	0.216%
20	18.157	2575	2579	2582	rBV	87495	129294	1.20%	0.112%
21	18.198	2582	2586	2594	rVB2	527611	761184	7.09%	0.657%
22	18.363	2608	2614	2618	rBV2	223202	369698	3.44%	0.319%
23	18.680	2663	2668	2671	rBV	88030	140825	1.31%	0.122%
24	19.245	2760	2764	2773	rVB4	63419	117705	1.10%	0.102%
25	19.375	2780	2786	2795	rBV	3752212	5200302	48.42%	4.491%
26	19.522	2807	2811	2816	rBV2	117526	186880	1.74%	0.161%
27	19.627	2827	2829	2834	rVB	105114	124821	1.16%	0.108%
28	19.722	2840	2845	2846	rBV	653272	752004	7.00%	0.649%
29	19.751	2846	2850	2855	rVB	3090790	4348113	40.49%	3.755%
30	19.939	2878	2882	2883	rBV2	200181	218051	2.03%	0.188%
31	19.975	2883	2888	2899	rVB	7905227	10739989	100.00%	9.275%
32	20.092	2902	2908	2909	rBV2	137618	245760	2.29%	0.212%
33	20.233	2929	2932	2934	rBV3	90987	130756	1.22%	0.113%
34	20.269	2934	2938	2944	rVB	551739	827922	7.71%	0.715%
35	20.375	2951	2956	2960	rBV2	474474	687692	6.40%	0.594%
36	20.433	2961	2966	2970	rVV3	291111	485247	4.52%	0.419%

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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-905-KJ-SO-0-0.5-081924-FD

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-BP081324.M
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37	20.474	2970	2973	2977	rVB2	138875	207563	1.93%	0.179%
38	20.580	2988	2991	2995	rVB2	122287	136422	1.27%	0.118%
39	20.633	2996	3000	3004	rVB3	129220	190263	1.77%	0.164%
40	21.263	3104	3107	3111	rVB	233537	311293	2.90%	0.269%
41	21.310	3112	3115	3119	rVB	271232	310019	2.89%	0.268%
42	21.374	3119	3126	3130	rBV2	718611	1409267	13.12%	1.217%
43	21.710	3175	3183	3188	rBV3	4263730	9883137	92.02%	8.535%
44	21.757	3188	3191	3201	rVB	1932508	3135186	29.19%	2.708%
45	21.916	3213	3218	3227	rBV	377411	631038	5.88%	0.545%
46	22.139	3252	3256	3265	rVB3	299768	588204	5.48%	0.508%
47	23.939	3557	3562	3572	rVB3	712694	1629658	15.17%	1.407%
48	24.063	3575	3583	3592	rBV	1596838	5062433	47.14%	4.372%
49	24.333	3625	3629	3634	rVB2	237665	430652	4.01%	0.372%
50	24.833	3707	3714	3727	rVB	899248	2538277	23.63%	2.192%
51	24.986	3732	3740	3752	rVB	1272636	3410862	31.76%	2.946%
52	25.139	3758	3766	3775	rBV	2061873	5706868	53.14%	4.928%

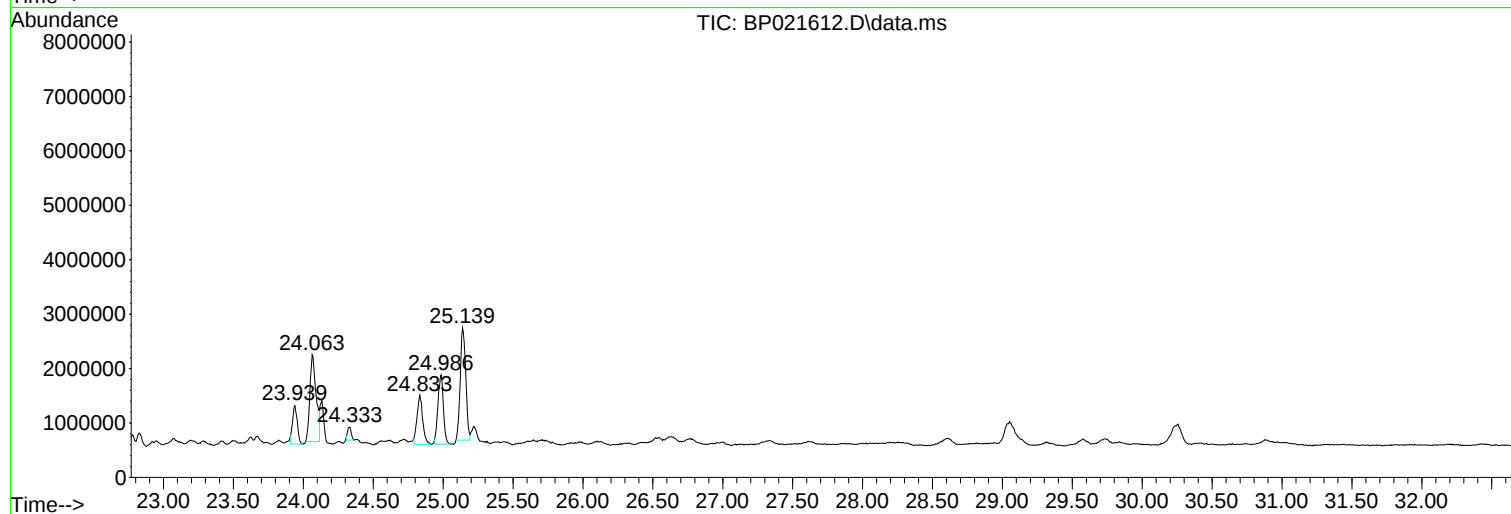
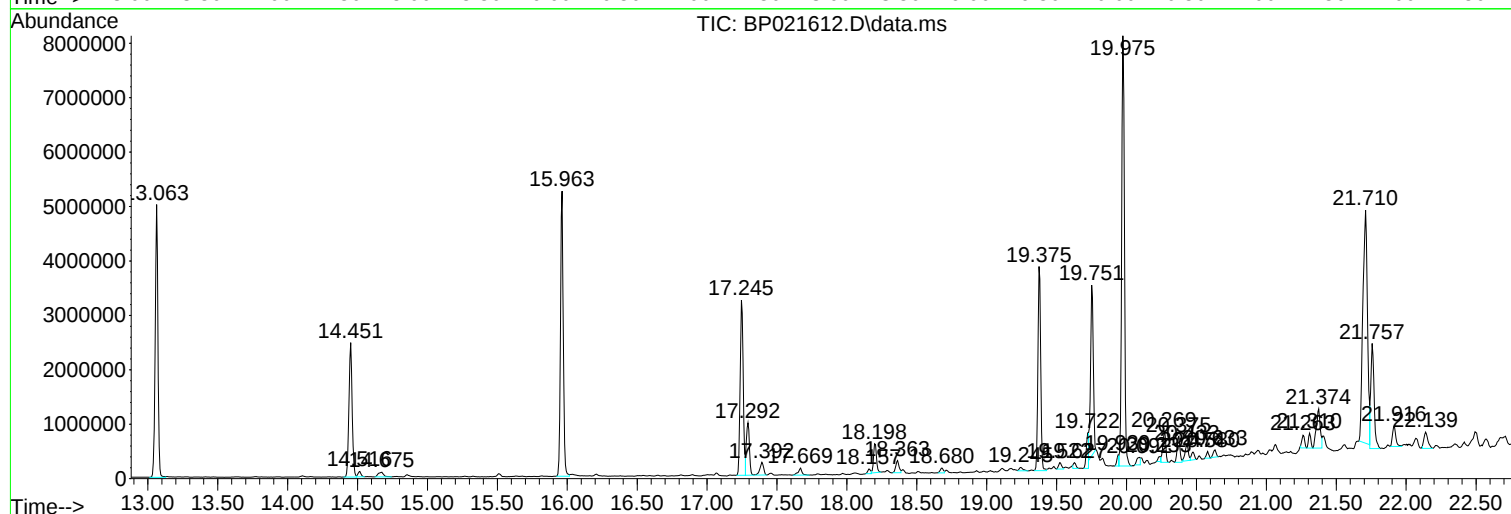
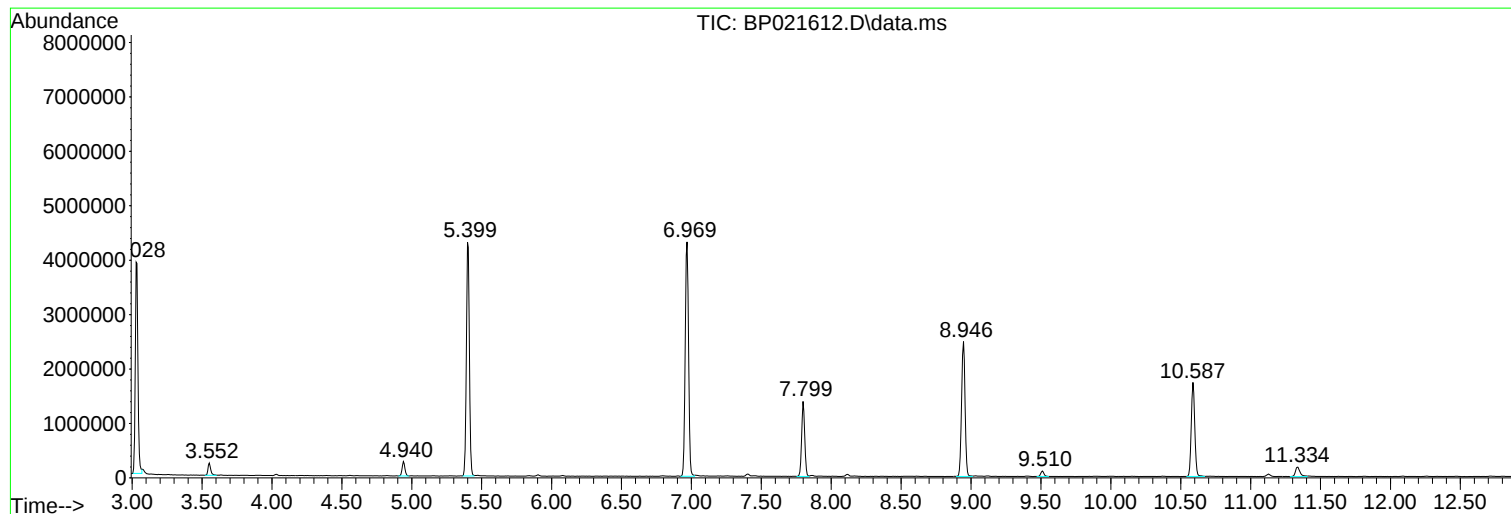
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 7 Sample Multiplier: 1

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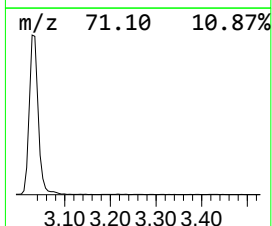
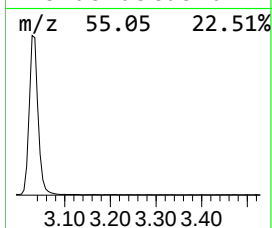
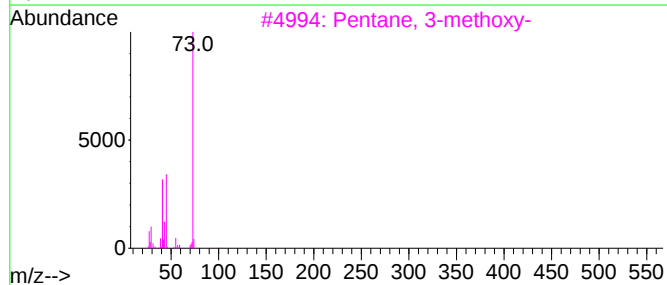
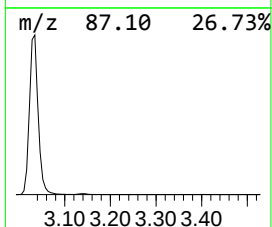
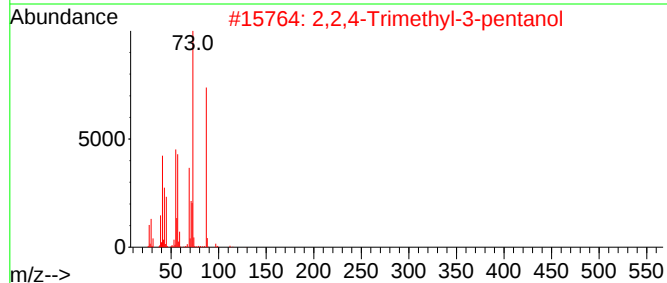
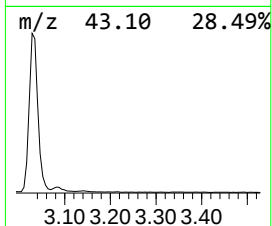
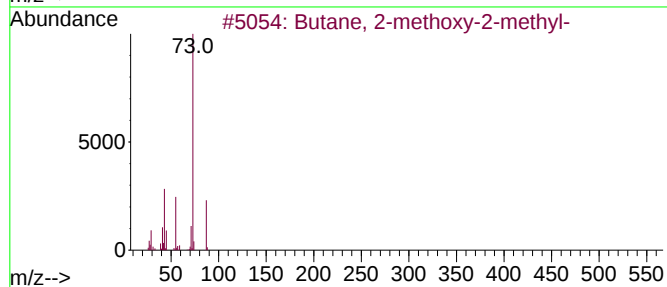
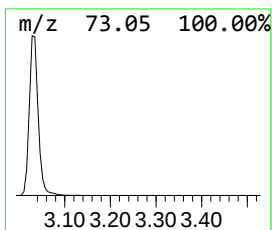
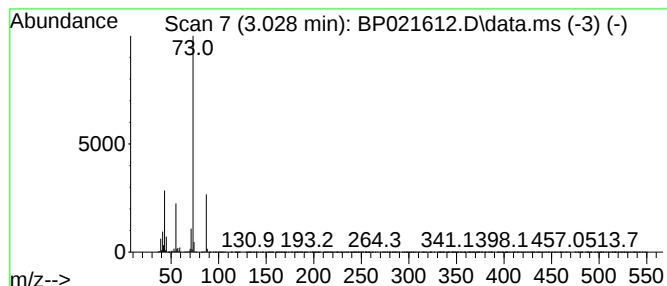
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	48.92 ng	5180510	1,4-Dichlorobenzene-d4	7.799

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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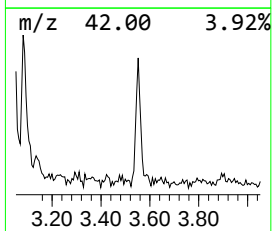
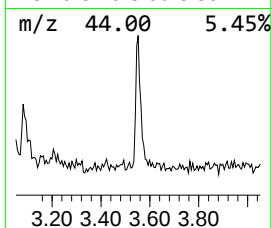
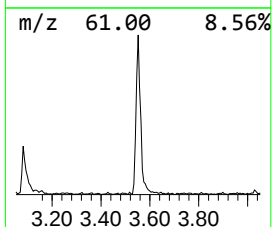
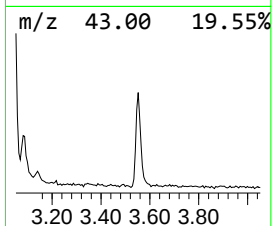
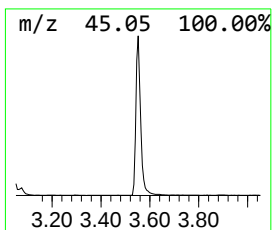
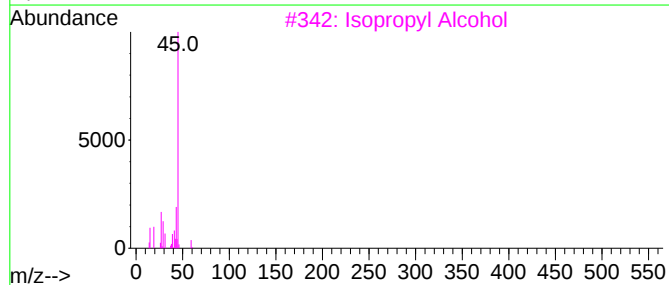
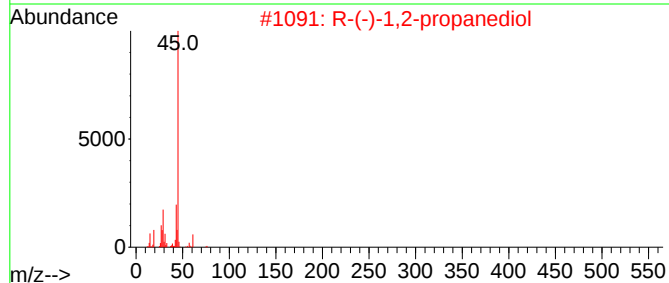
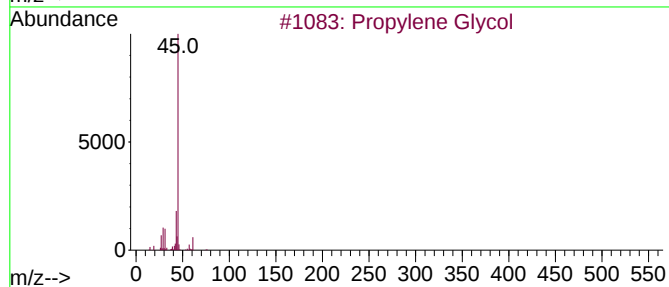
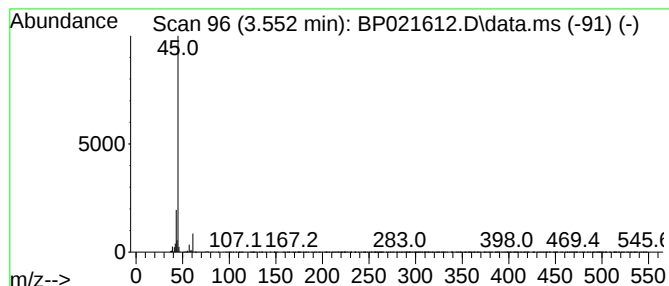
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.552	2.94 ng	311672	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	83
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	40
4			Formamide	45	CH3NO	000075-12-7	5
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-905-KJ-SO-0-0.5-081924-FD

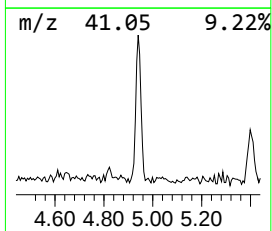
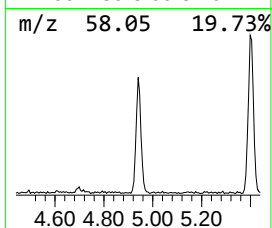
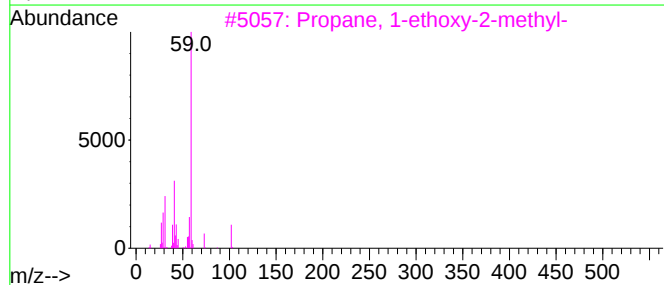
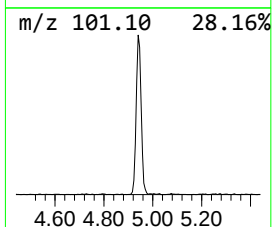
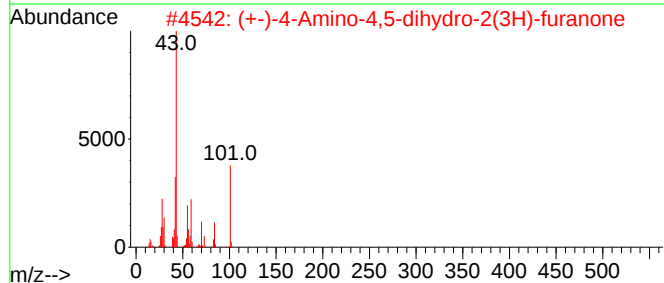
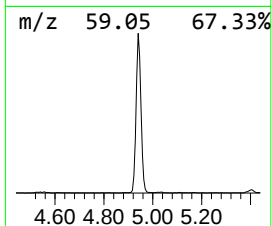
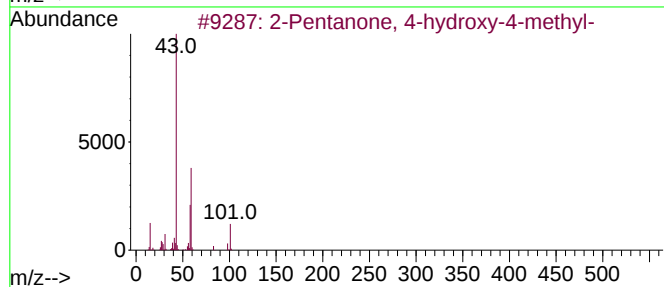
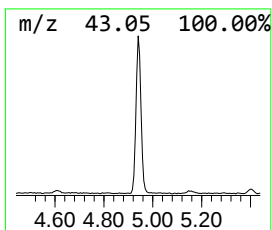
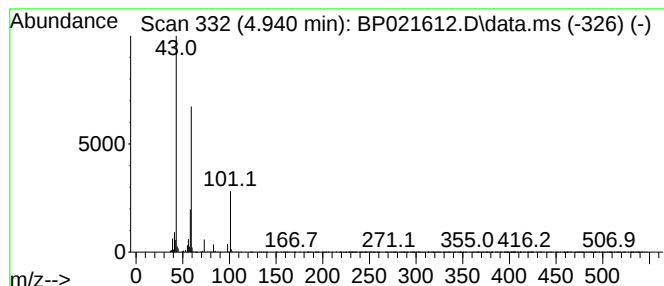
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	3.53 ng	374295	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27
4			2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	14



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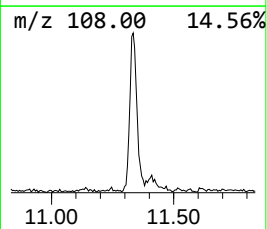
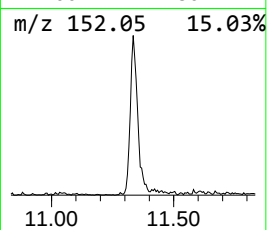
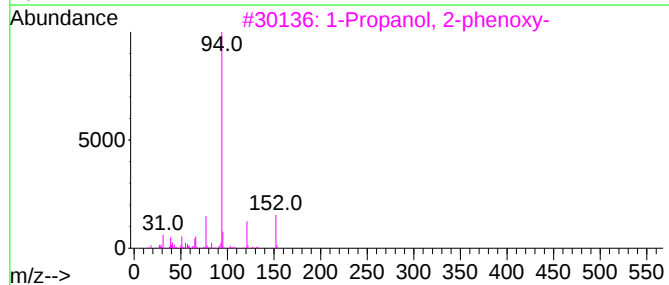
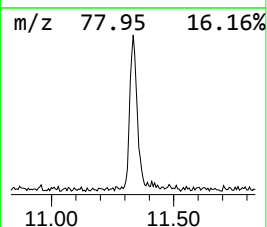
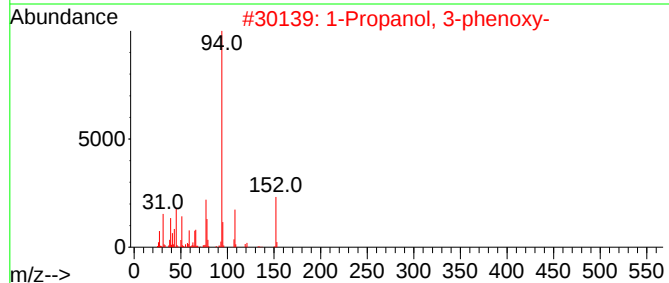
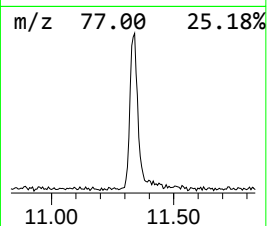
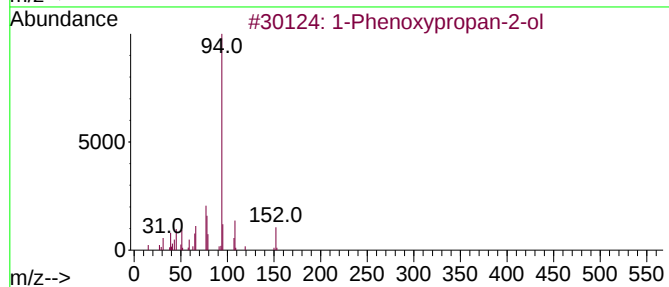
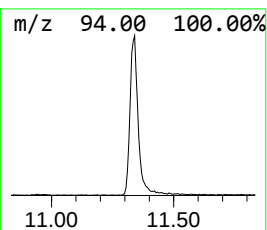
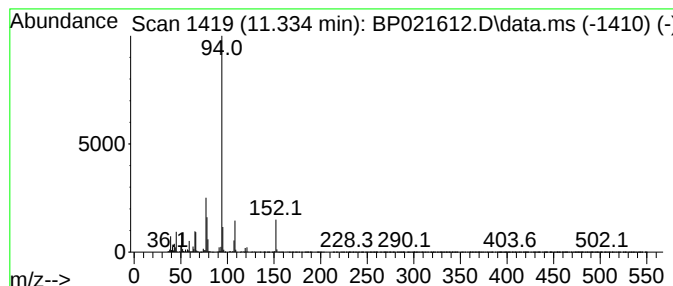
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.334	2.79 ng	415267	Naphthalene-d8	10.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			Benzene, propoxy-	136	C9H12O	000622-85-5	53



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S-905-KJ-SO-0-0.5-081924-FD

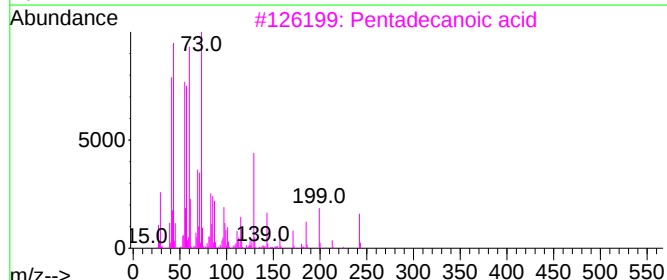
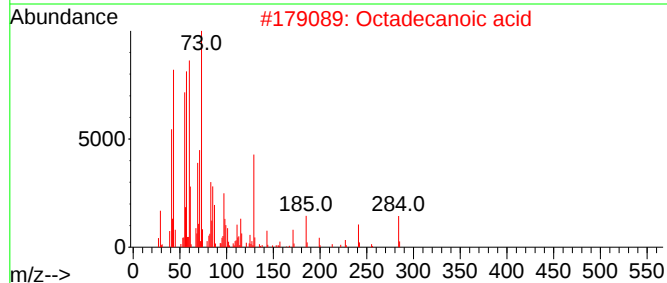
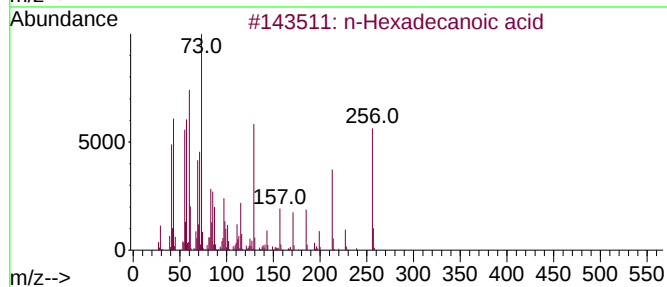
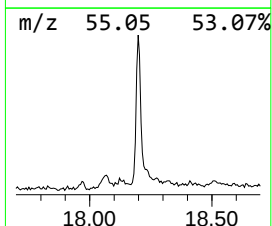
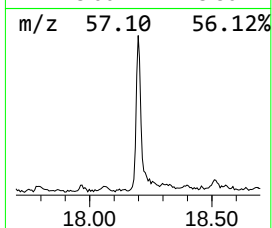
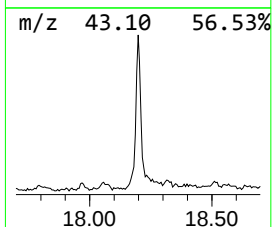
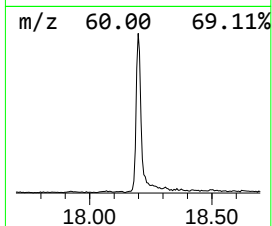
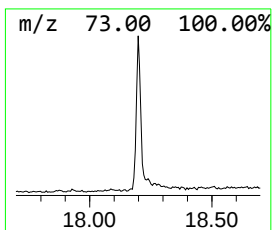
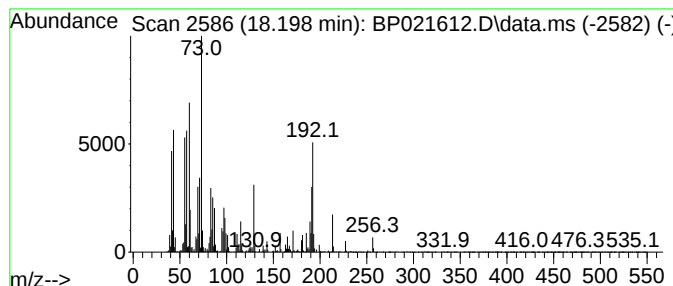
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	3.08 ng	761184	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	60
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021612.D
Acq On : 22 Aug 2024 13:39
Operator : RC/JU
Sample : P3671-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-905-KJ-SO-0-0.5-081924-FD

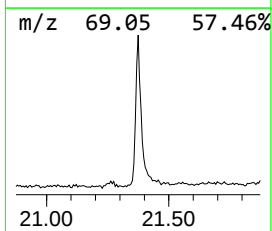
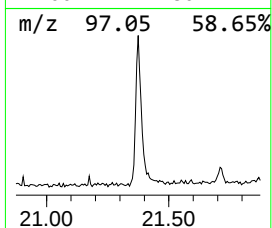
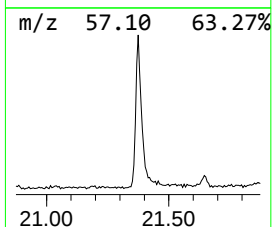
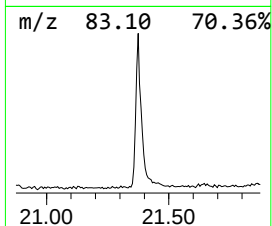
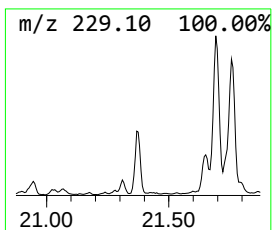
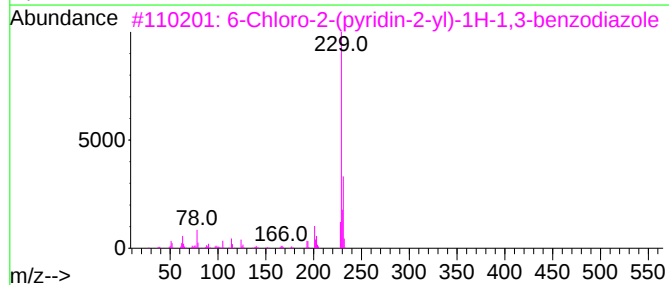
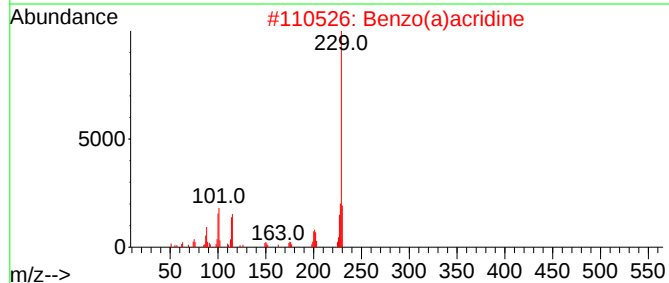
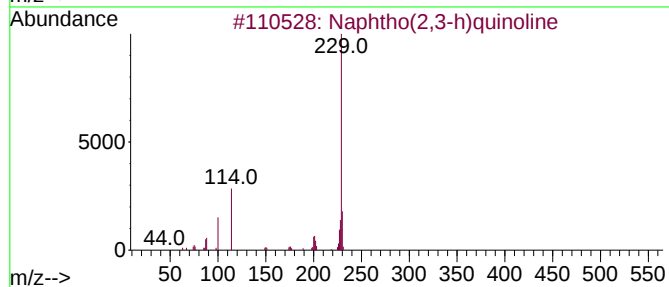
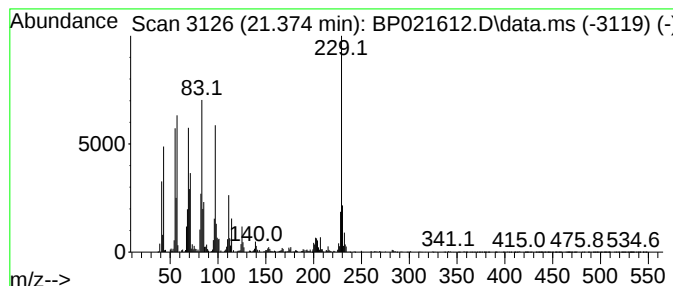
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown21.374 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.374	2.85 ng	1409270	Chrysene-d12	21.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphtho(2,3-h)quinoline	229	C17H11N	000084-56-0	38
2			Benzo(a)acridine	229	C17H11N	000225-11-6	30
3			6-Chloro-2-(pyridin-2-yl)-1H-1,3...	229	C12H8ClN3	063053-15-6	27
4			Silane, methylvinyl(1-cyclohexyl)...	312	C18H36O2Si	1000421-14-5	27
5			Malononitrile, 2-indeno[1,2-b]py...	229	C15H7N3	1000316-60-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021612.D
Acq On : 22 Aug 2024 13:39
Operator : RC/JU
Sample : P3671-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-905-KJ-SO-0-0.5-081924-FD

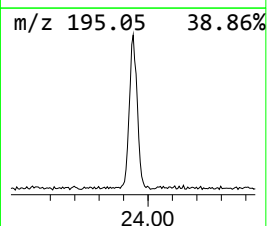
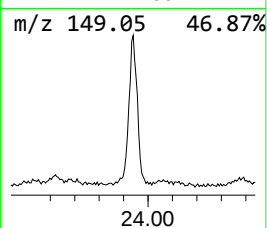
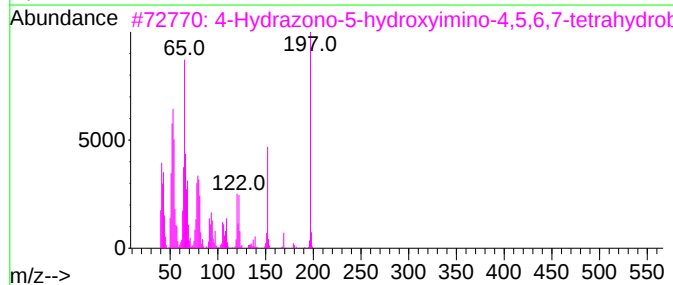
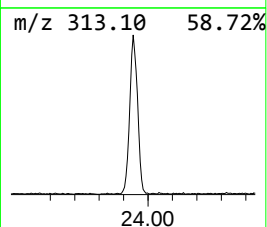
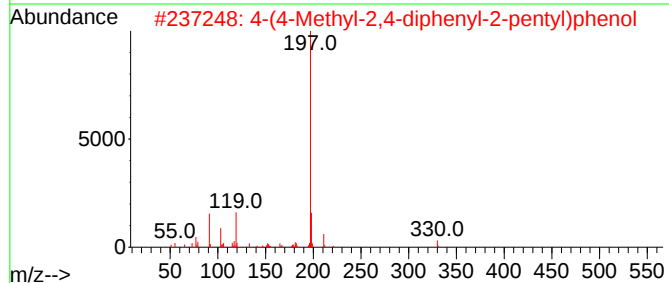
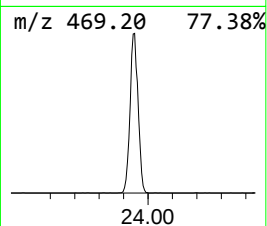
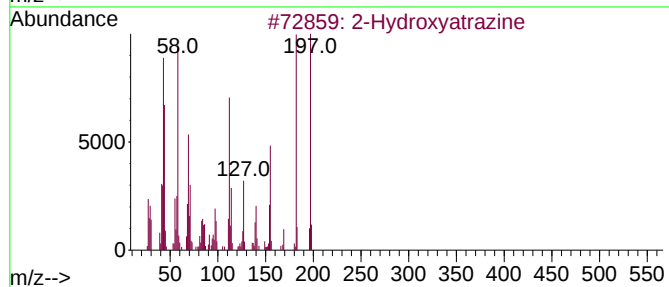
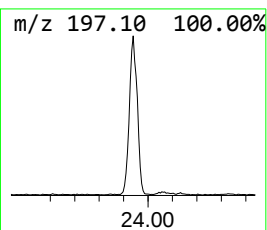
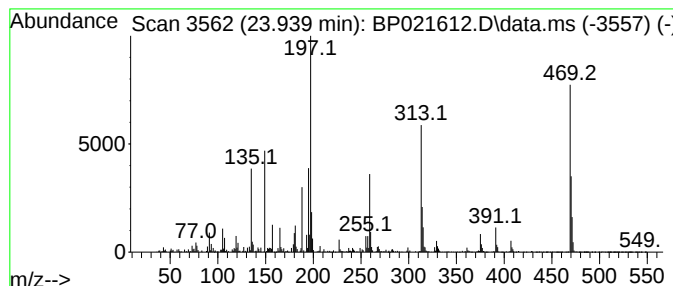
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown23.939 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.939	5.71 ng	1629660	Perylene-d12	25.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hydroxyatrazine	197	C8H15N5O	002163-68-0	25
2			4-(4-Methyl-2,4-diphenyl-2-penty...	330	C24H26O	052379-26-7	15
3			4-Hydrazono-5-hydroxyimino-4,5,6...	197	C6H7N5O3	303194-86-7	11
4			p,p'-Ditolylamine	197	C14H15N	000620-93-9	11
5			Pentanamide, 5-chloro-N-(2'-benz...	315	C18H18ClNO2	163064-46-8	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021612.D
Acq On : 22 Aug 2024 13:39
Operator : RC/JU
Sample : P3671-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-905-KJ-SO-0-0.5-081924-FD

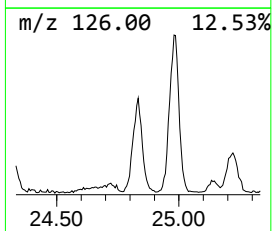
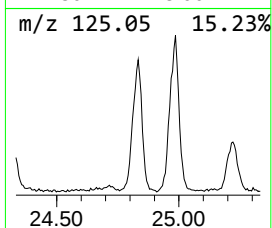
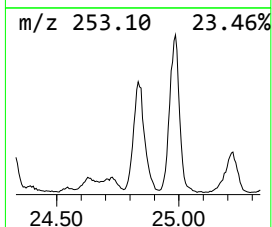
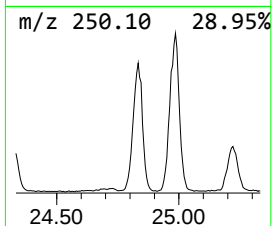
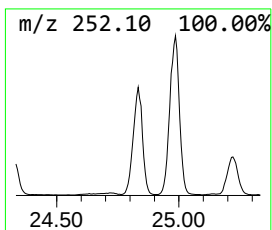
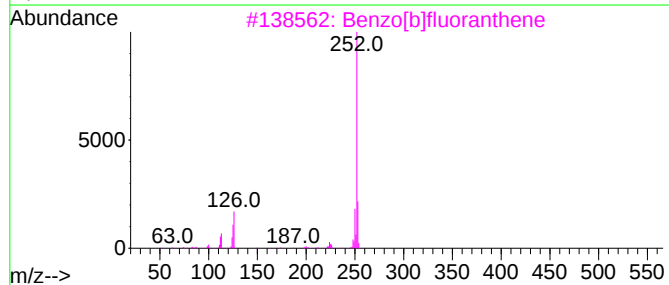
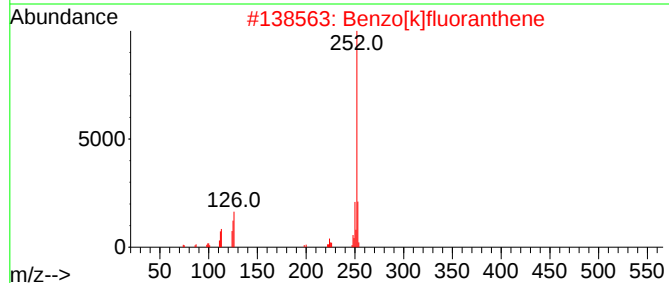
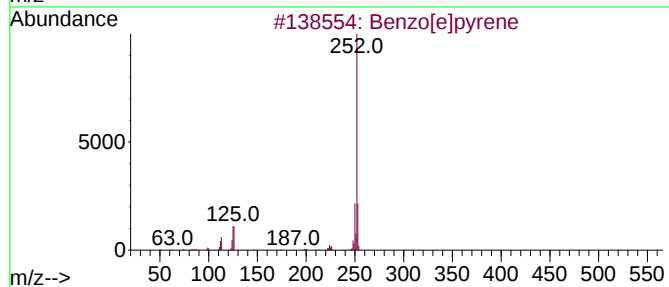
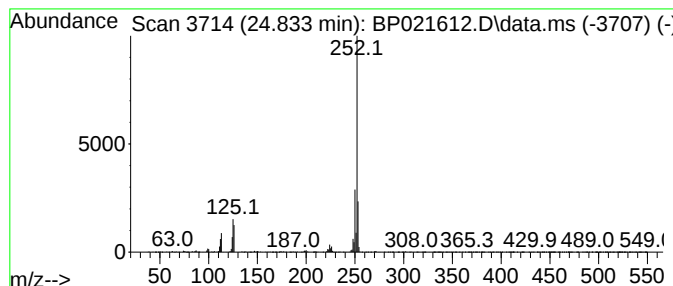
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.833	8.90 ng	2538280	Perylene-d12	25.139

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021612.D
Acq On : 22 Aug 2024 13:39
Operator : RC/JU
Sample : P3671-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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...	3.028	48.9	ng	5180510	1	7.799	2117910	20.0
Propylene Glycol	3.552	2.9	ng	311672	1	7.799	2117910	20.0
2-Pentanone, 4-...	4.940	3.5	ng	374295	1	7.799	2117910	20.0
1-Phenoxypropan...	11.334	2.8	ng	415267	2	10.587	2977680	20.0
n-Hexadecanoic ...	18.198	3.1	ng	761184	4	17.245	4949490	20.0
unknown21.374	21.374	2.9	ng	1409270	5	21.716	9883140	20.0
unknown23.939	23.939	5.7	ng	1629660	6	25.139	5706870	20.0
Benzo[e]pyrene	24.833	8.9	ng	2538280	6	25.139	5706870	20.0