

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
 Data File : BP019825.D
 Acq On : 22 Feb 2024 15:32
 Operator : MA/JU
 Sample : P1537-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 9

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-BP013124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	322	328	338	rVB	185562	272662	9.50%	1.309%
2	5.469	398	405	417	rBV	733258	1123711	39.13%	5.394%
3	7.069	670	677	693	rBV	671263	1116483	38.88%	5.359%
4	7.893	811	817	826	rBV	211568	347962	12.12%	1.670%
5	9.063	1007	1016	1030	rBV	419401	753188	26.23%	3.615%
6	10.692	1285	1293	1307	rBV	254252	464031	16.16%	2.227%
7	13.157	1703	1712	1734	rBV	1153691	1838758	64.03%	8.826%
8	13.428	1753	1758	1765	rVB	24043	40250	1.40%	0.193%
9	14.257	1893	1899	1906	rBV	49120	85465	2.98%	0.410%
10	14.528	1938	1945	1953	rBV	413862	655846	22.84%	3.148%
11	14.592	1953	1956	1961	rVB2	20899	31334	1.09%	0.150%
12	14.757	1975	1984	1990	rBV	290145	656884	22.88%	3.153%
13	15.145	2044	2050	2055	rBV4	16288	34322	1.20%	0.165%
14	15.580	2120	2124	2135	rVB3	22918	53304	1.86%	0.256%
15	16.028	2193	2200	2214	rBV	1112813	1719042	59.86%	8.251%
16	16.257	2234	2239	2248	rVB10	21385	46892	1.63%	0.225%
17	16.592	2290	2296	2300	rBV6	16257	32757	1.14%	0.157%
18	16.951	2353	2357	2362	rVB3	20821	37607	1.31%	0.181%
19	17.110	2380	2384	2391	rVB	26953	44192	1.54%	0.212%
20	17.292	2409	2415	2418	rBV	511702	792376	27.59%	3.803%
21	17.333	2418	2422	2428	rVB	328995	483578	16.84%	2.321%
22	17.422	2433	2437	2442	rVB	107798	158679	5.53%	0.762%
23	17.869	2510	2513	2520	rVB2	31230	55464	1.93%	0.266%
24	18.157	2558	2562	2564	rBV	116314	154669	5.39%	0.742%
25	18.186	2564	2567	2575	rVB2	242928	497812	17.34%	2.389%
26	18.286	2581	2584	2589	rVB	51516	54900	1.91%	0.264%
27	18.345	2589	2594	2598	rVV2	146773	278124	9.69%	1.335%
28	18.380	2598	2600	2605	rVB	92889	107967	3.76%	0.518%
29	18.645	2641	2645	2650	rBV	66391	99438	3.46%	0.477%
30	18.927	2691	2693	2696	rVB2	36411	33772	1.18%	0.162%
31	19.045	2709	2713	2717	rBV	108091	159621	5.56%	0.766%
32	19.186	2733	2737	2743	rBV5	70880	123105	4.29%	0.591%
33	19.298	2752	2756	2762	rBV	750909	1021116	35.56%	4.901%
34	19.651	2808	2816	2824	rVB	734071	1235846	43.04%	5.932%
35	19.857	2846	2851	2862	rVB	2296043	2871552	100.00%	13.783%
36	20.474	2953	2956	2962	rBV	87147	127929	4.46%	0.614%

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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-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.104	3060	3063	3070	rVB2	249726	363471	12.66%	1.745%
38	21.380	3104	3110	3114	rBV2	825126	1596602	55.60%	7.664%
39	21.421	3115	3117	3124	rVB	401661	494425	17.22%	2.373%
40	23.804	3518	3522	3529	rVB	391988	768185	26.75%	3.687%

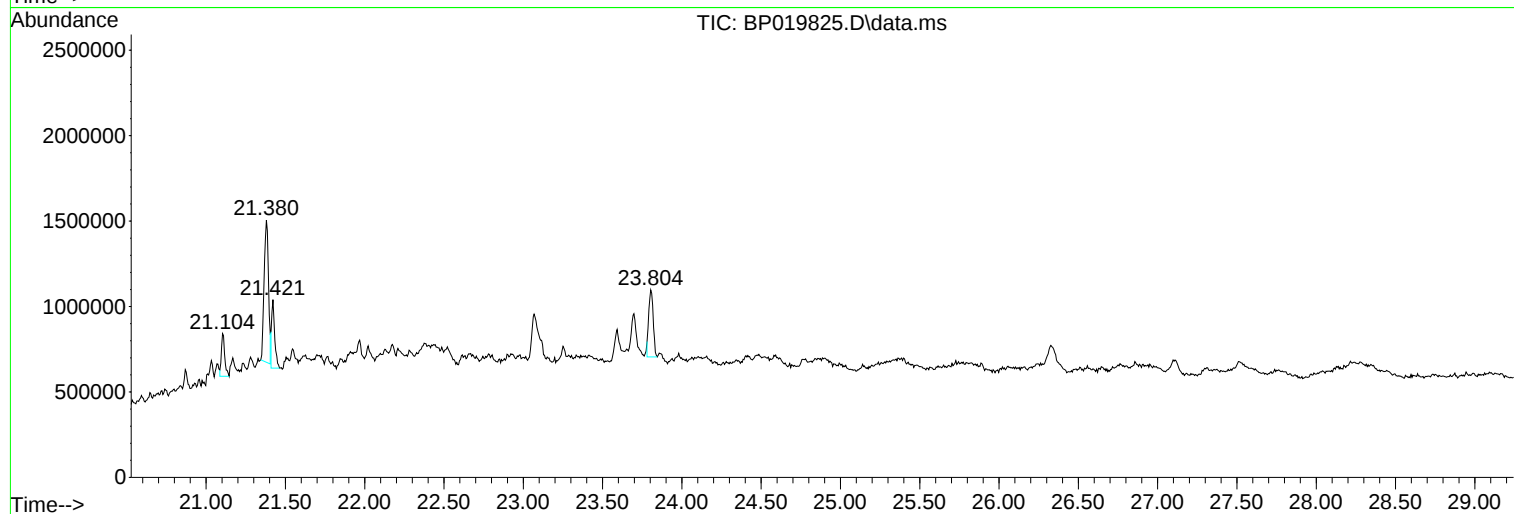
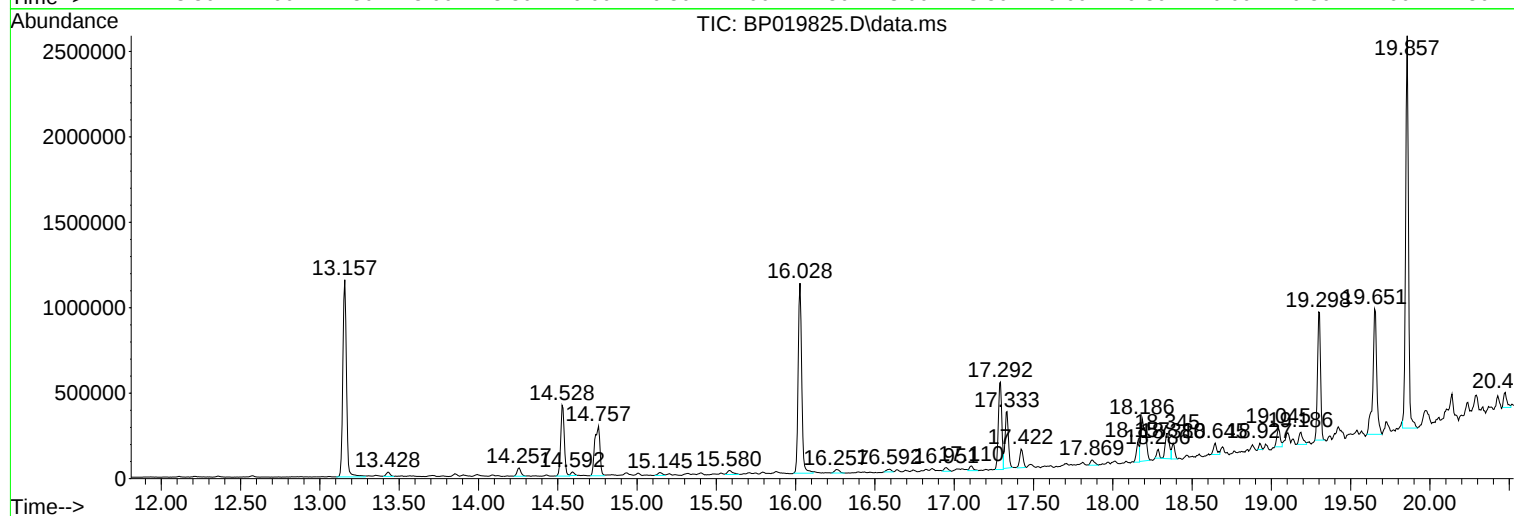
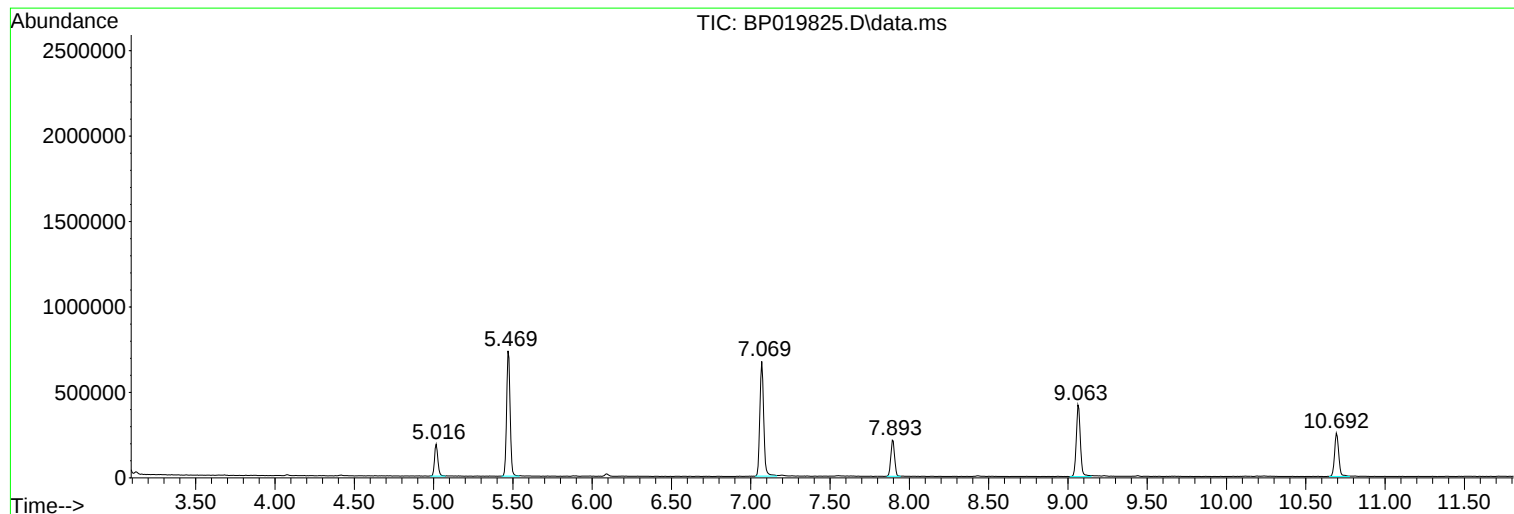
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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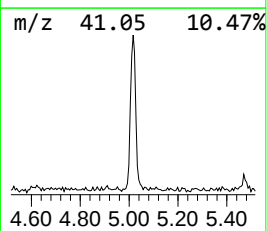
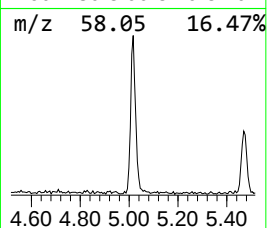
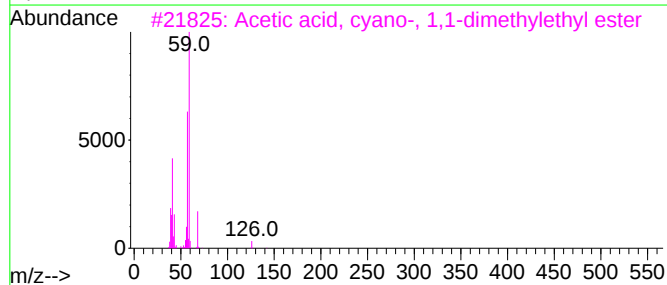
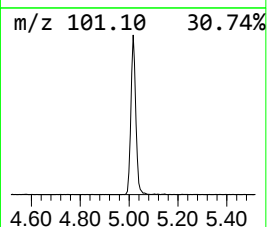
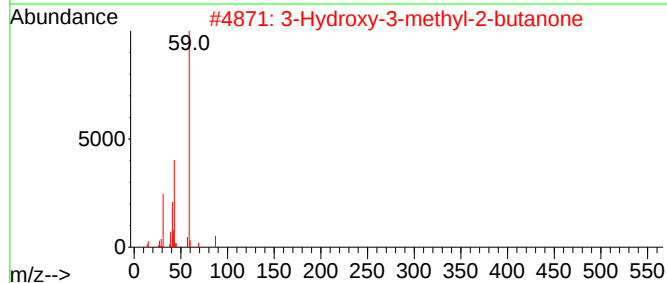
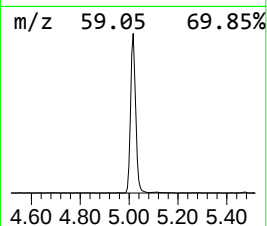
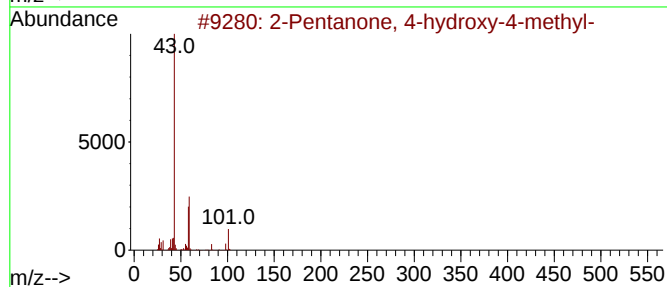
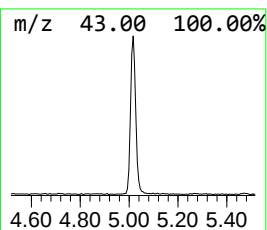
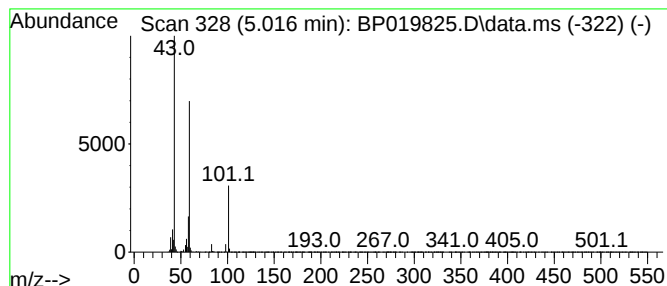
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	15.67 ng	272662	1,4-Dichlorobenzene-d4	7.899

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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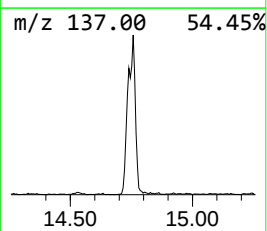
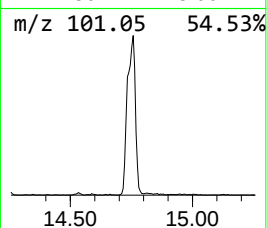
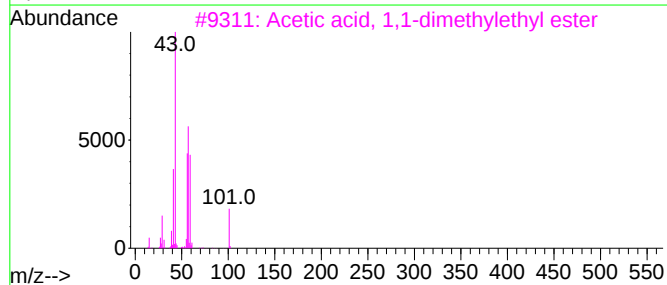
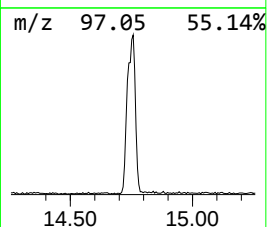
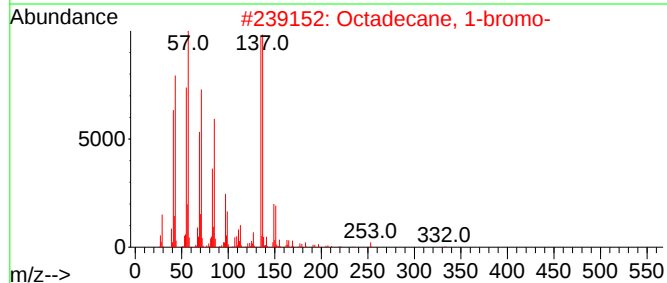
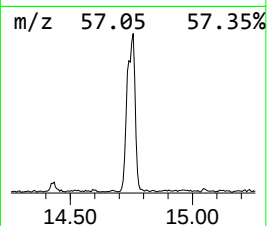
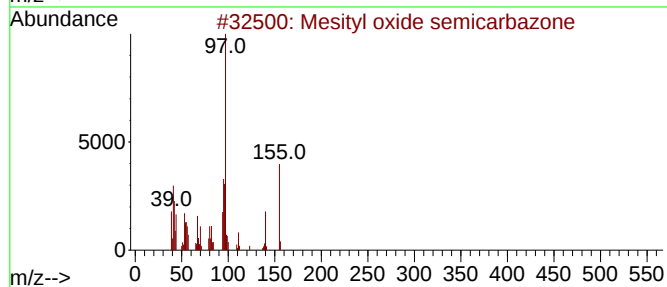
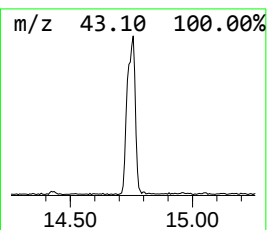
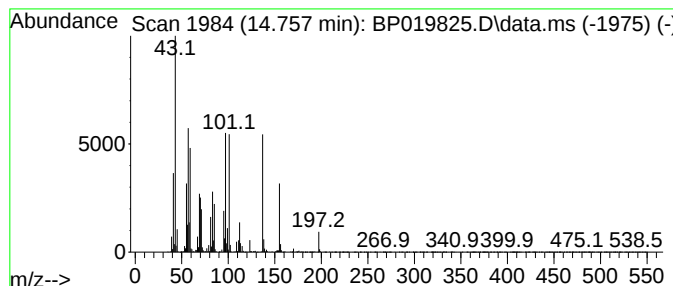
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown14.757 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	20.03 ng	656884	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesityl oxide semicarbazone	155	C7H13N3O	003780-62-9	22
2			Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	18
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
4			Succinic acid, cyclohexylmethyl ...	284	C16H28O4	1000370-90-1	12
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11



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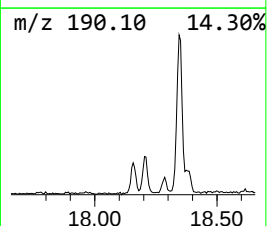
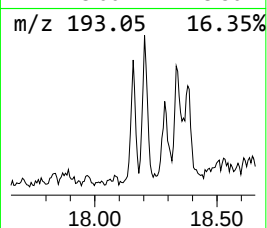
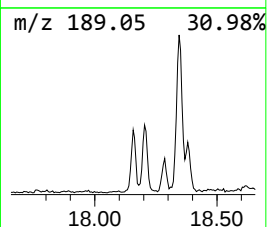
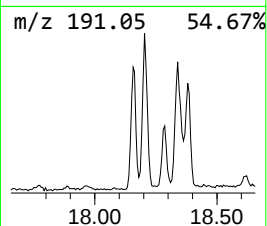
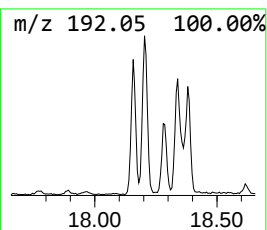
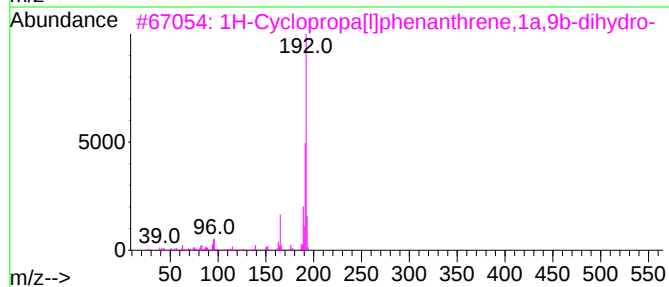
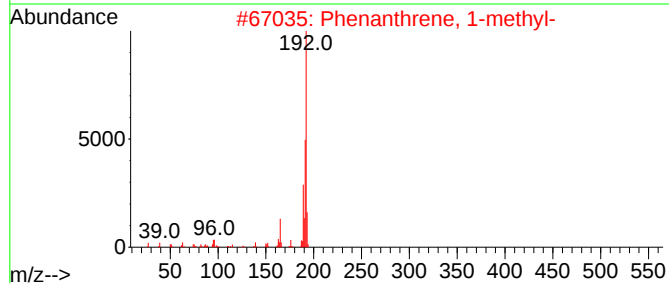
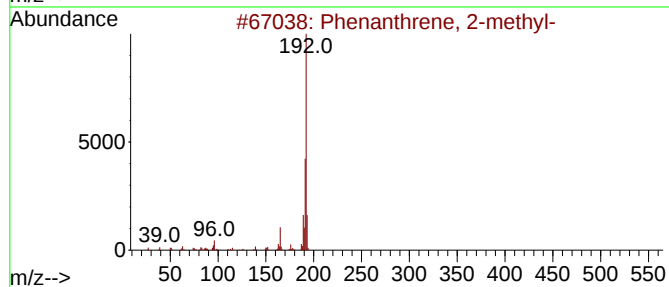
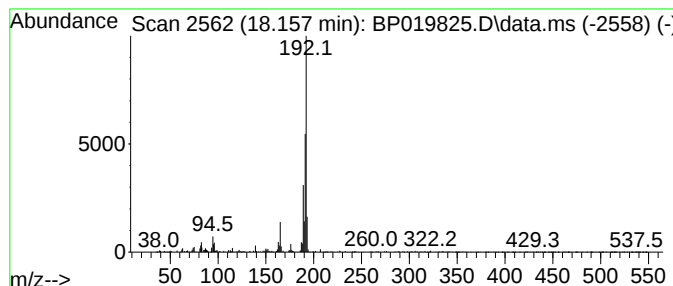
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	3.90 ng	154669	Phenanthrene-d10	17.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
3		1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
4		Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	94



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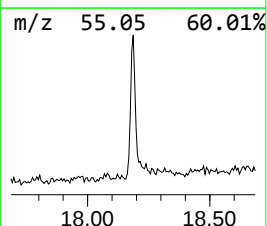
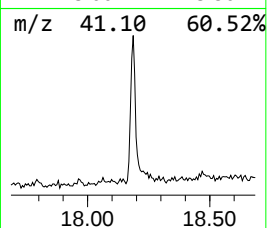
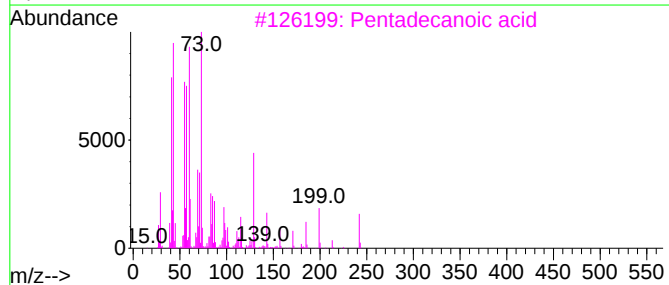
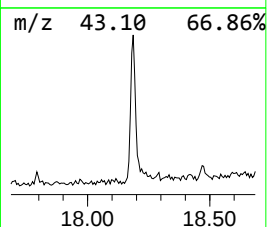
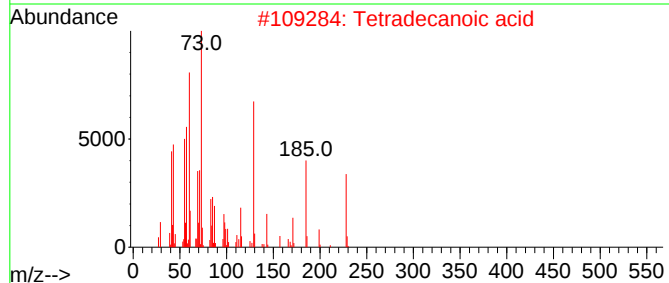
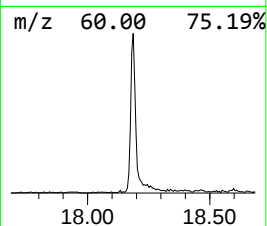
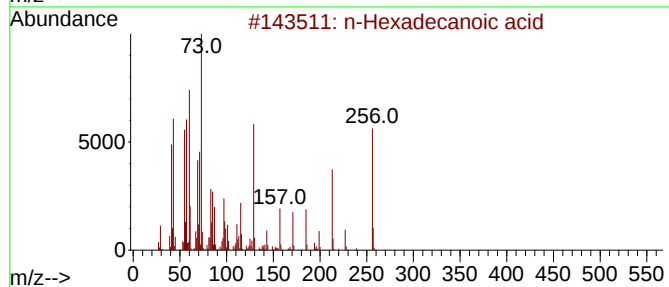
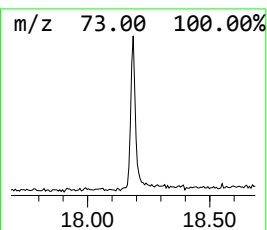
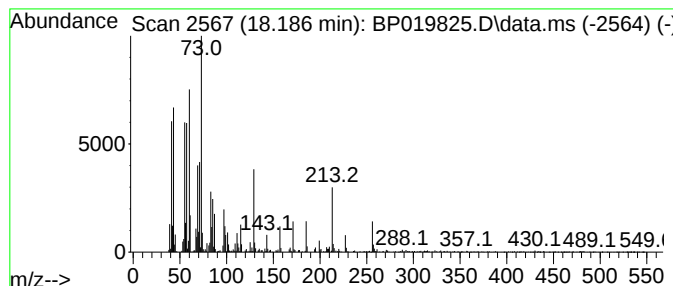
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	12.57 ng	497812	Phenanthrene-d10	17.292

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	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Octadecanoic acid	284	C18H36O2	000057-11-4	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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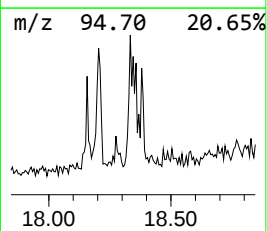
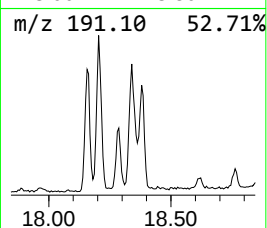
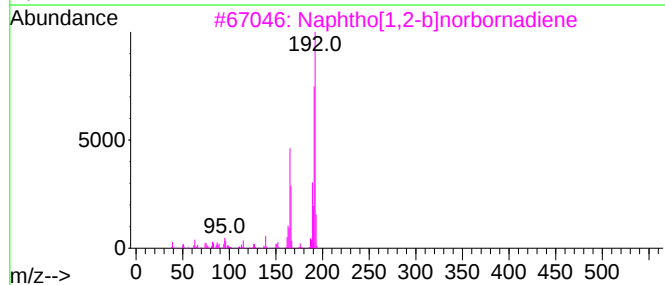
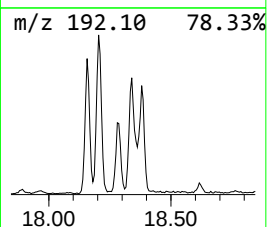
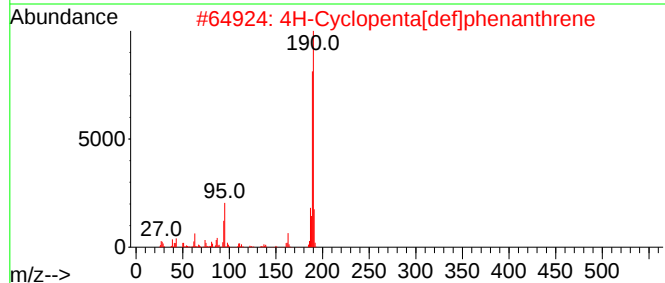
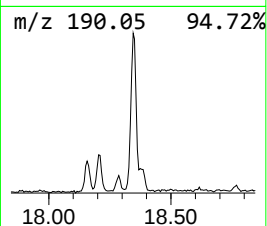
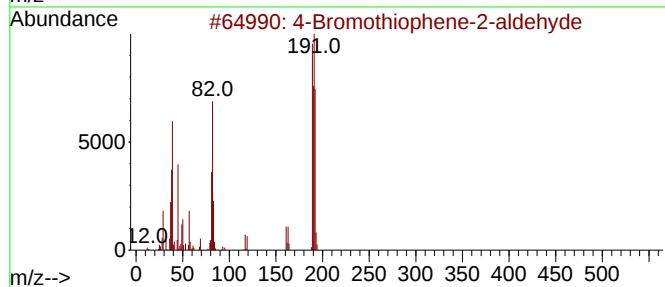
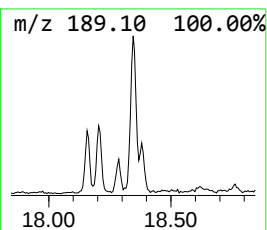
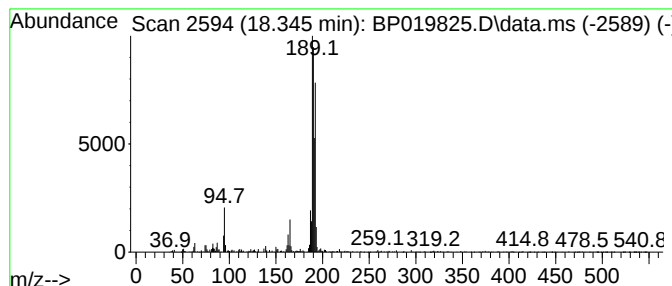
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4-Bromothiophene-2-aldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	7.02 ng	278124	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	58
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
3			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	46
4			Dodecanoic acid, 2,2,2-trichloro...	330	C14H25Cl3O2	1000360-54-3	43
5			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019825.D
Acq On : 22 Feb 2024 15:32
Operator : MA/JU
Sample : P1537-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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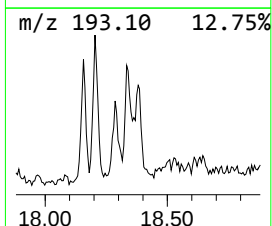
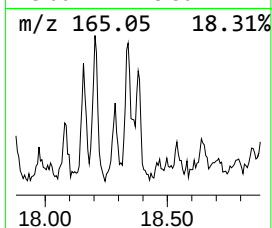
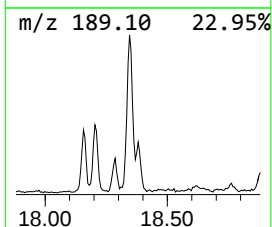
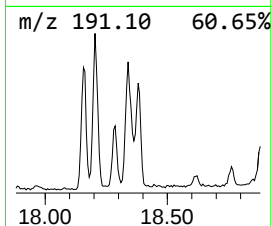
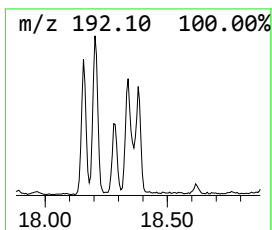
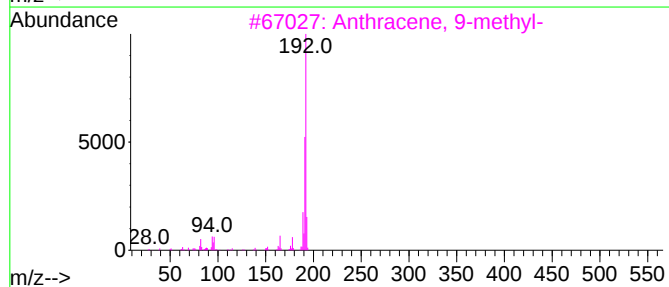
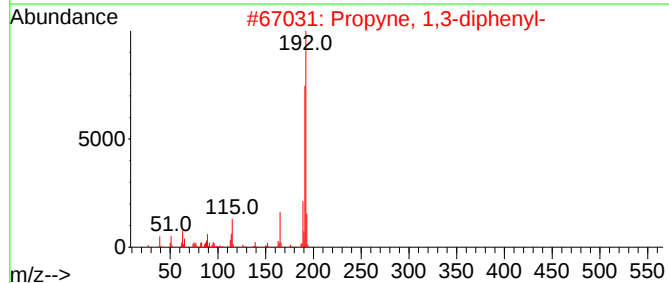
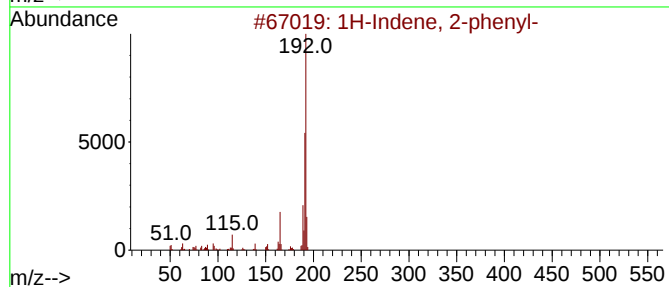
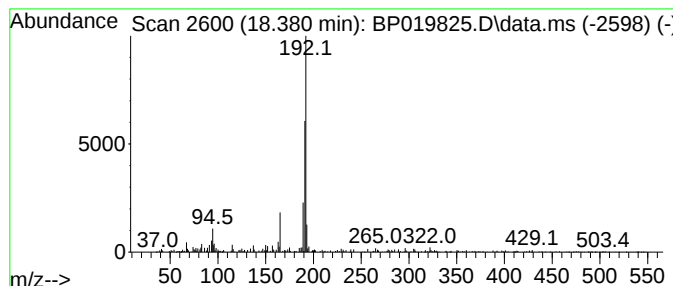
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1H-Indene, 2-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.380	2.73 ng	107967	Phenanthrene-d10	17.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	76
2		Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	76
3		Anthracene, 9-methyl-	192	C15H12	000779-02-2	72
4		Anthracene, 2-methyl-	192	C15H12	000613-12-7	68
5		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019825.D
Acq On : 22 Feb 2024 15:32
Operator : MA/JU
Sample : P1537-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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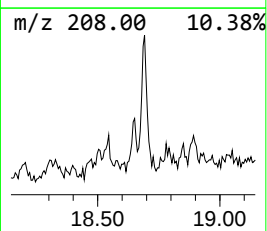
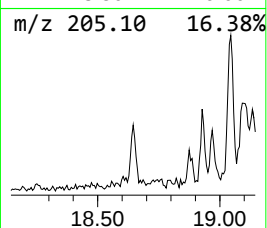
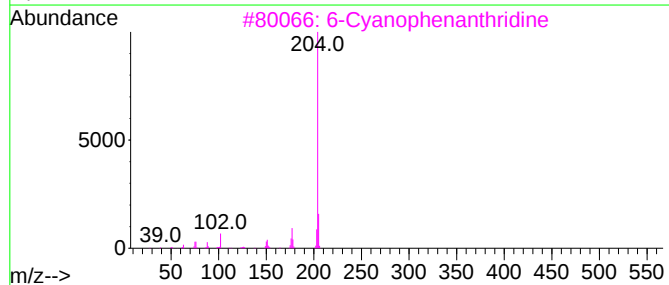
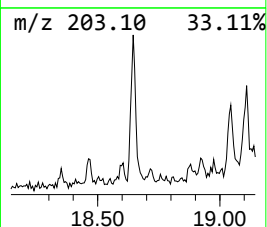
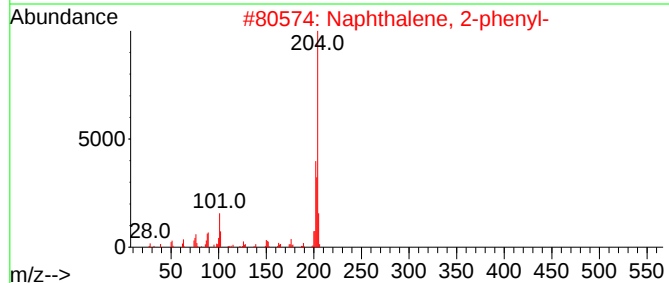
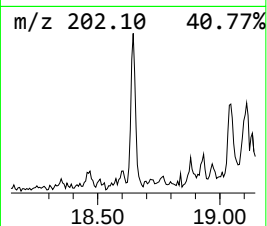
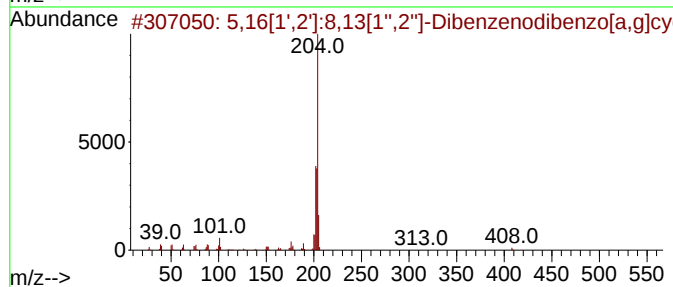
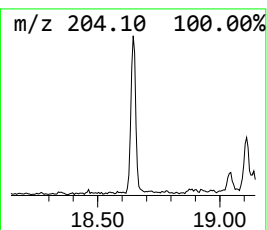
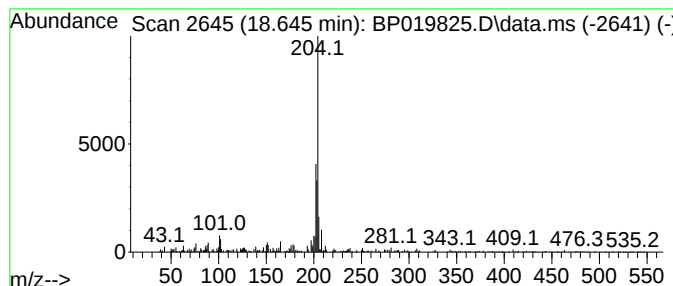
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5,16[1',2']:8,13[1'',2'']-D... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.645	2.51 ng	99438	Phenanthrene-d10	17.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	80	
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	60	
3	6-Cyanophenanthridine	204	C14H8N2	002176-28-5	55	
4	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	49	
5	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	49	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019825.D
Acq On : 22 Feb 2024 15:32
Operator : MA/JU
Sample : P1537-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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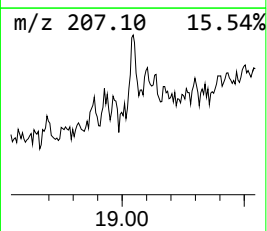
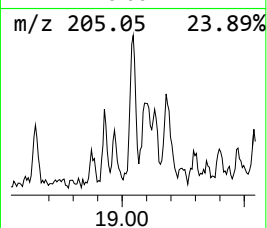
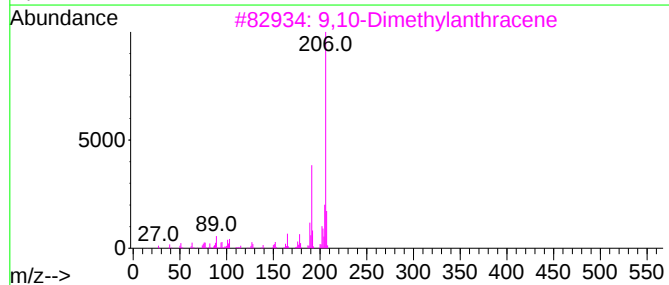
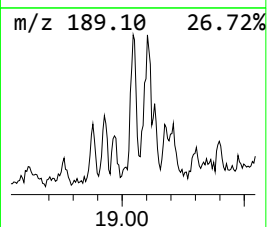
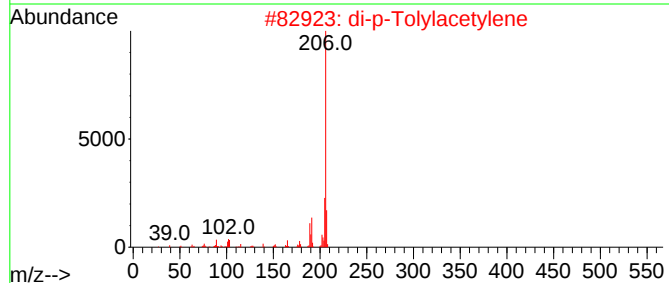
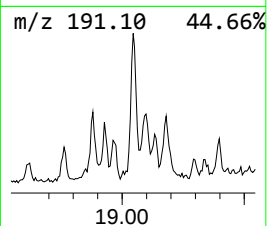
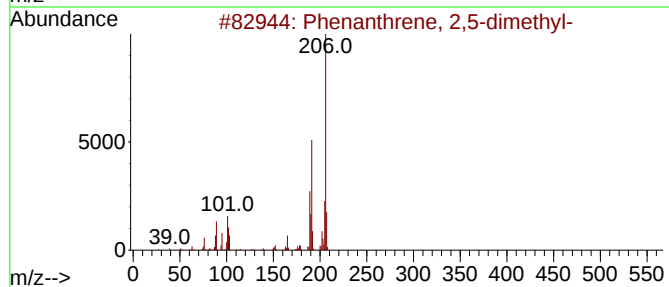
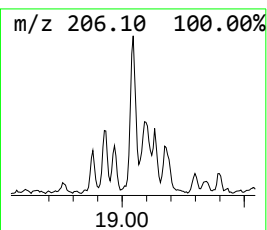
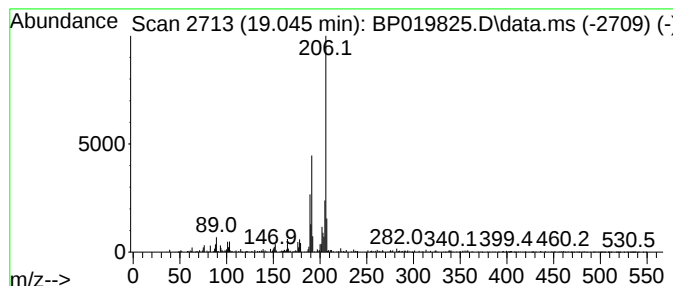
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.045	4.03 ng	159621	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2			di-p-Tolylacetylene	206	C16H14	002789-88-0	91
3			9,10-Dimethylantracene	206	C16H14	000781-43-1	91
4			Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	87
5			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019825.D
Acq On : 22 Feb 2024 15:32
Operator : MA/JU
Sample : P1537-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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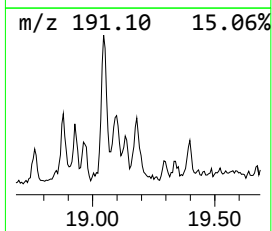
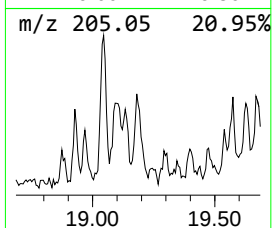
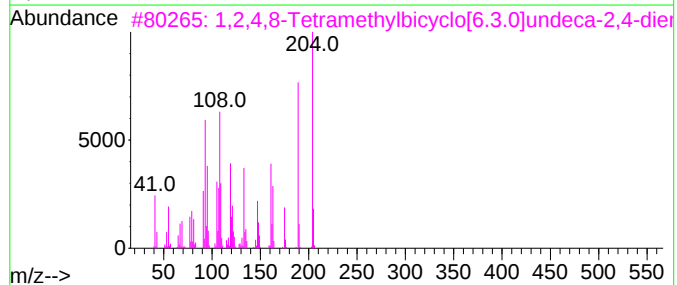
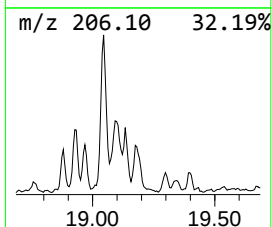
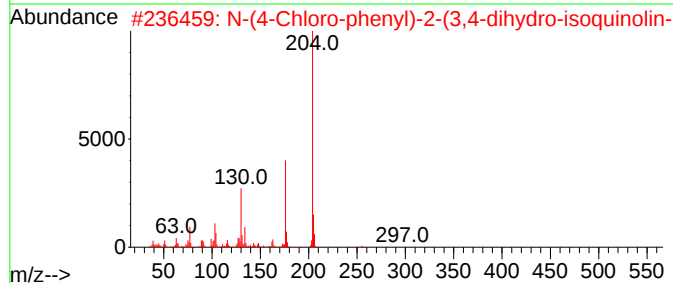
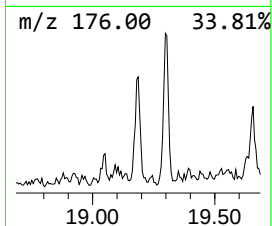
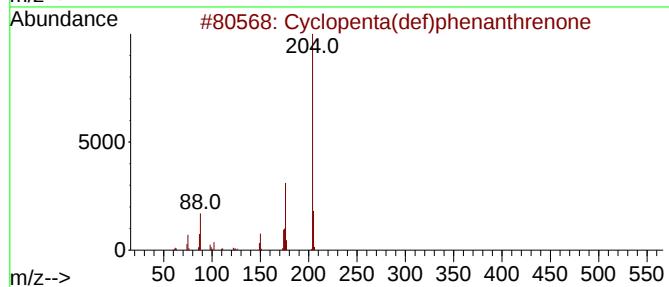
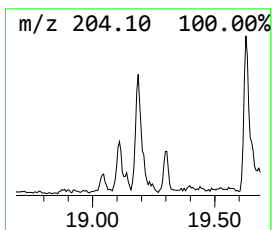
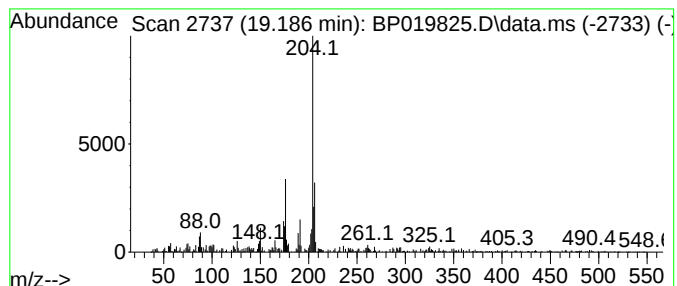
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopenta(def)phenanthrenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.186	3.11 ng	123105	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	90
2			N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1010296-34-3	64
3			1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	64
4			[1,1'-Biphenyl]-2-ol, 5-chloro-	204	C12H9ClO	000607-12-5	59
5			2-Chloro-3-chloromethyl-5,7-dime...	239	C12H11Cl2N	948290-59-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019825.D
Acq On : 22 Feb 2024 15:32
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Sample : P1537-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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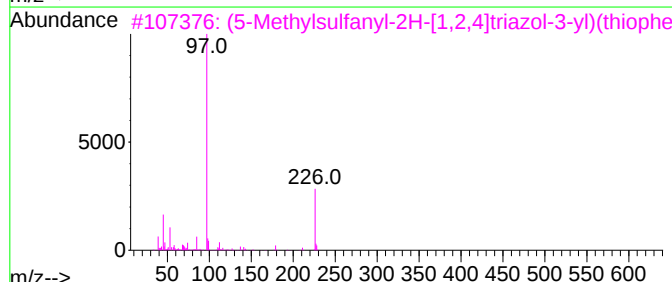
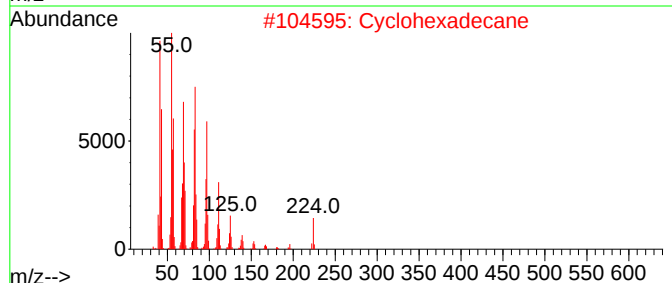
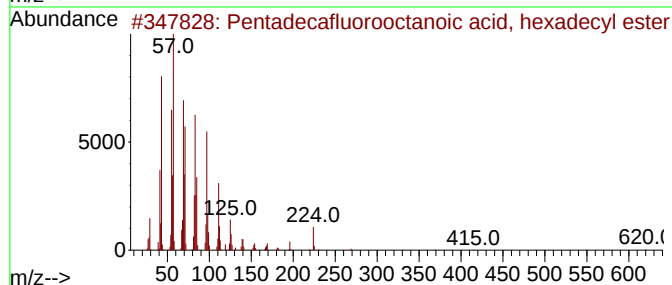
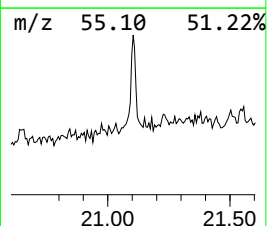
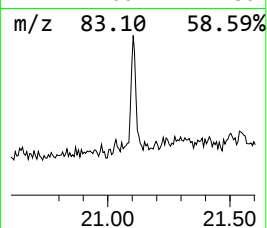
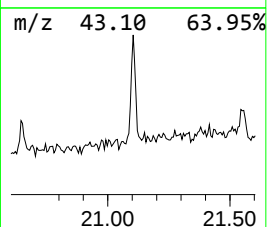
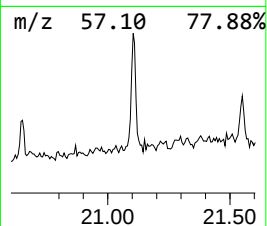
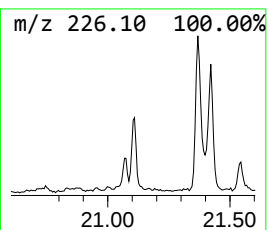
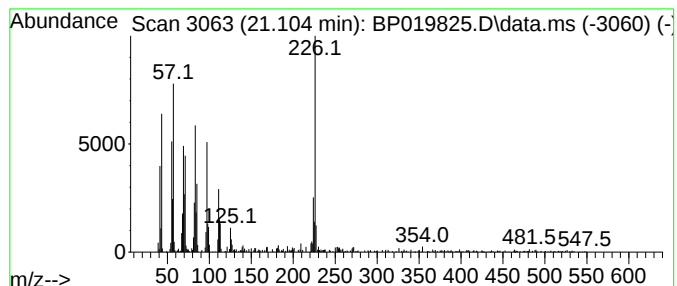
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	4.55 ng	363471	Chrysene-d12	21.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	78
2		Cyclohexadecane	224	C16H32	000295-65-8	50
3		(5-Methylsulfonyl-2H-[1,2,4]tria...	226	C8H10N4S2	1000316-82-0	35
4		Valeramide, 2-methyl-N-(2-phenyl...	415	C28H49NO	1000491-52-3	35
5		Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019825.D
Acq On : 22 Feb 2024 15:32
Operator : MA/JU
Sample : P1537-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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-...	5.016	15.7	ng	272662	1	7.899	347962	20.0
unknown14.757	14.757	20.0	ng	656884	3	14.534	655846	20.0
Phenanthrene, 2...	18.157	3.9	ng	154669	4	17.292	792376	20.0
n-Hexadecanoic ...	18.186	12.6	ng	497812	4	17.292	792376	20.0
4-Bromothiophen...	18.345	7.0	ng	278124	4	17.292	792376	20.0
1H-Indene, 2-ph...	18.380	2.7	ng	107967	4	17.292	792376	20.0
5,16[1',2']:8,1...	18.645	2.5	ng	99438	4	17.292	792376	20.0
Phenanthrene, 2...	19.045	4.0	ng	159621	4	17.292	792376	20.0
Cyclopenta(def)...	19.186	3.1	ng	123105	4	17.292	792376	20.0
Pentadecafluoro...	21.104	4.5	ng	363471	5	21.386	1596600	20.0