

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101921\
 Data File : BF125907.D
 Acq On : 19 Oct 2021 19:00
 Operator : JU/CG
 Sample : M4259-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1-BS

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_F\METHODS\8270-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125907.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.439	565	570	573	rBV	2556321	2483110	86.85%	10.915%
2	6.451	737	742	745	rBV	2723035	2446032	85.56%	10.752%
3	6.822	802	805	809	rBV	1073119	861715	30.14%	3.788%
4	7.381	896	900	903	rBV	1807218	1528390	53.46%	6.718%
5	8.004	1003	1006	1019	rBV	218256	187757	6.57%	0.825%
6	8.104	1019	1023	1026	rBV	1467577	1154259	40.37%	5.074%
7	9.180	1202	1206	1209	rBV	3274700	2859004	100.00%	12.567%
8	9.716	1294	1297	1302	rBV	135890	116929	4.09%	0.514%
9	9.857	1317	1321	1324	rBV	1492081	1192321	41.70%	5.241%
10	10.398	1411	1413	1420	rVB	35282	42168	1.47%	0.185%
11	10.639	1450	1454	1458	rBV	1757119	1595618	55.81%	7.014%
12	11.233	1553	1555	1561	rVB2	36499	39387	1.38%	0.173%
13	11.339	1569	1573	1575	rBV	1402378	1135187	39.71%	4.990%
14	11.363	1575	1577	1580	rVV	316051	235868	8.25%	1.037%
15	11.410	1580	1585	1588	rVB	94740	99875	3.49%	0.439%
16	11.445	1588	1591	1594	rBV2	34062	34678	1.21%	0.152%
17	11.569	1609	1612	1614	rBV	48046	44123	1.54%	0.194%
18	11.839	1655	1658	1660	rBV	42322	43541	1.52%	0.191%
19	11.863	1660	1662	1667	rVB2	137932	136582	4.78%	0.600%
20	11.951	1673	1677	1680	rBV2	105210	115454	4.04%	0.507%
21	12.074	1695	1698	1701	rBV2	29324	31924	1.12%	0.140%
22	12.163	1710	1713	1716	rVB2	31430	42810	1.50%	0.188%
23	12.268	1728	1731	1733	rBV	36415	38065	1.33%	0.167%
24	12.392	1749	1752	1754	rBV	62327	62702	2.19%	0.276%
25	12.427	1754	1758	1760	rBV5	38301	52143	1.82%	0.229%
26	12.551	1775	1779	1782	rBV	539796	479396	16.77%	2.107%
27	12.645	1792	1795	1798	rBV2	113589	118083	4.13%	0.519%
28	12.774	1814	1817	1820	rBV	465155	414688	14.50%	1.823%
29	12.921	1839	1842	1846	rBV	2903315	2564329	89.69%	11.272%
30	13.104	1871	1873	1877	rVB2	115559	104933	3.67%	0.461%
31	13.974	2016	2021	2024	rBV2	1205329	1288347	45.06%	5.663%
32	13.998	2024	2025	2028	rVB	209164	126603	4.43%	0.556%
33	15.004	2194	2196	2199	rBV	168516	199557	6.98%	0.877%
34	15.362	2255	2257	2264	rVB	177868	188337	6.59%	0.828%
35	15.427	2264	2268	2271	rBV	590159	686169	24.00%	3.016%

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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_F\METHODS\8270-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

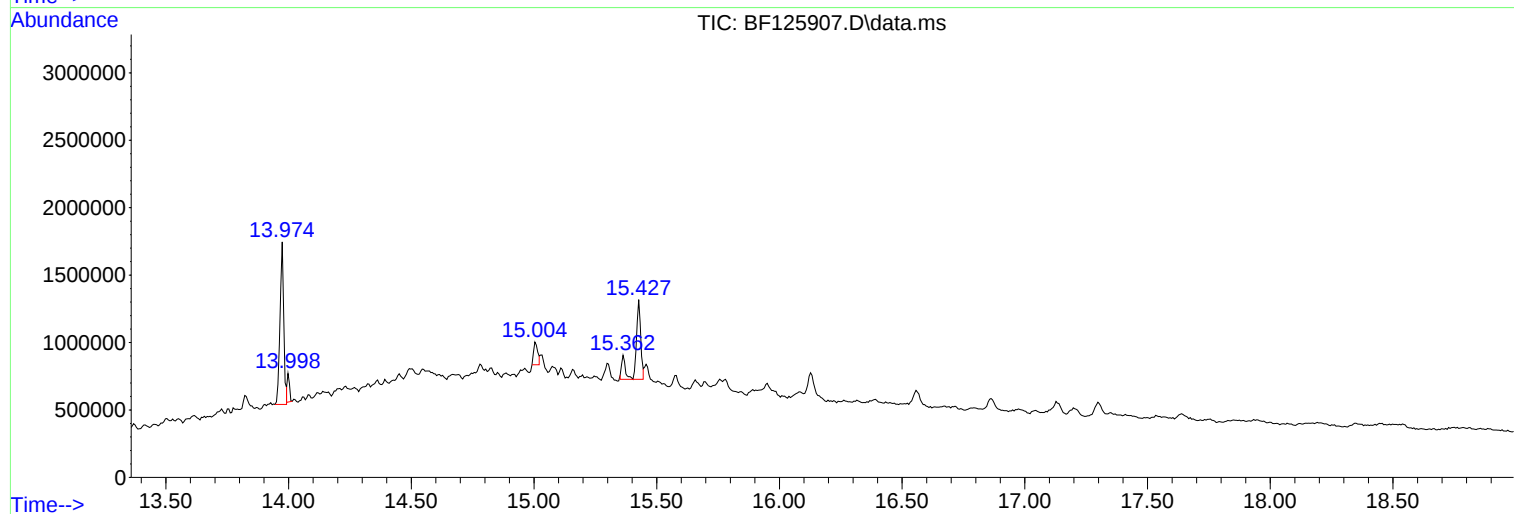
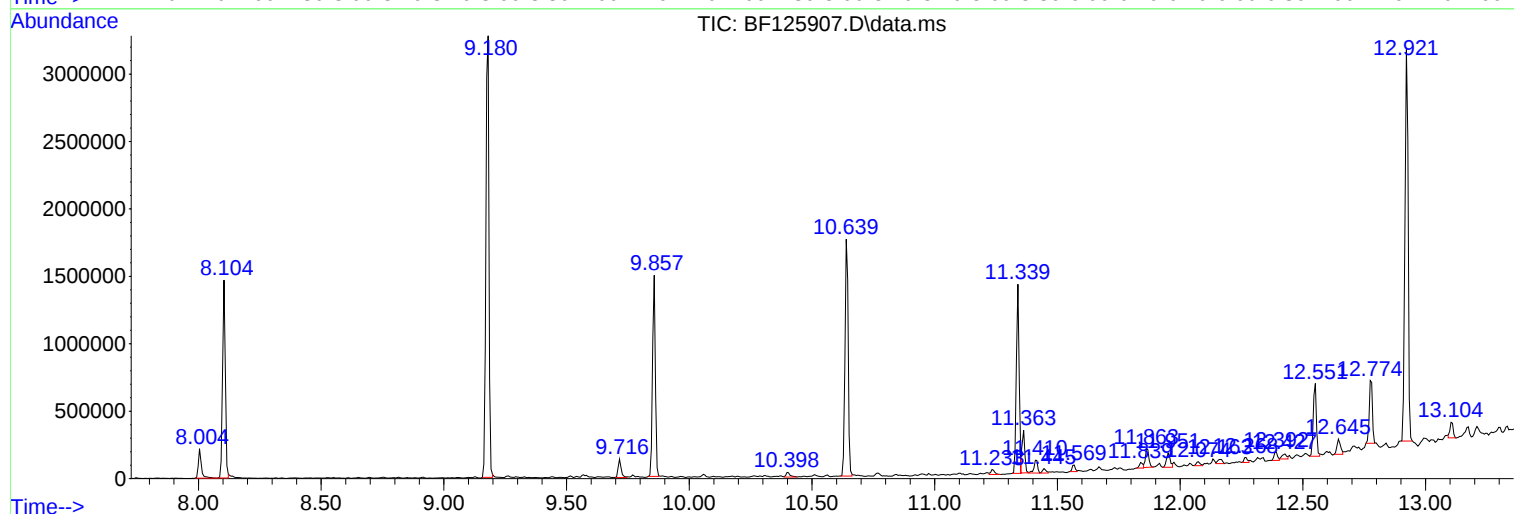
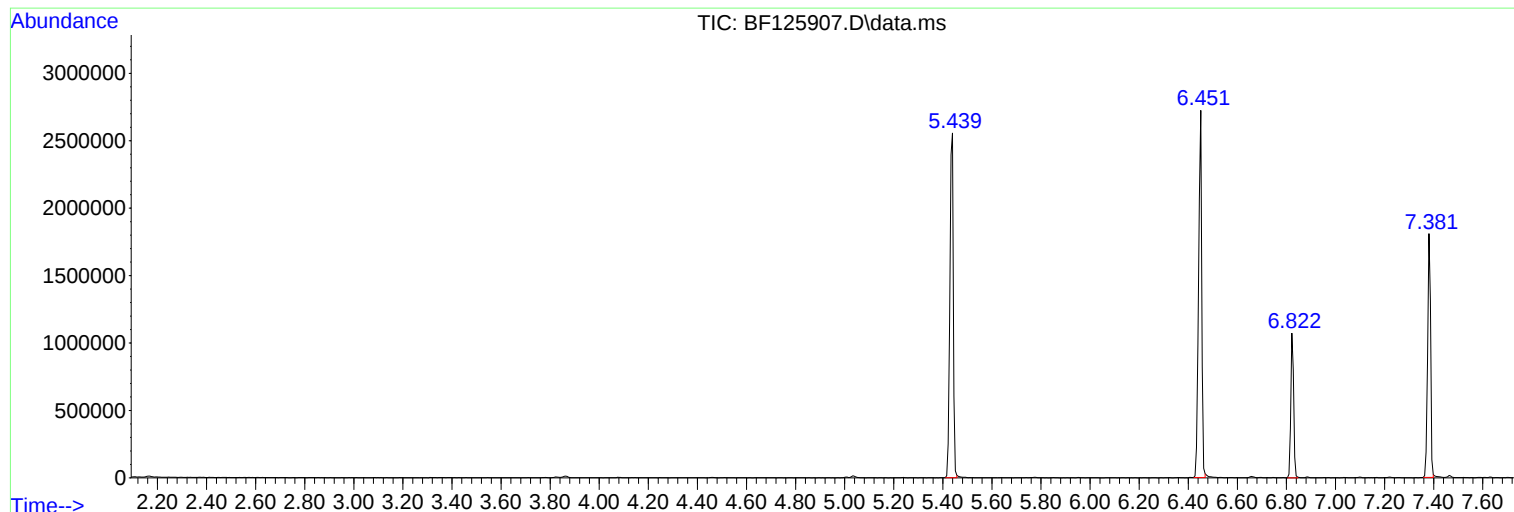
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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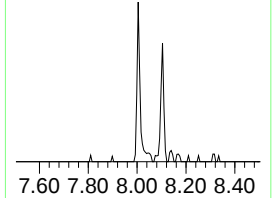
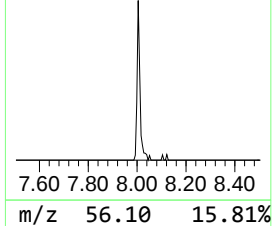
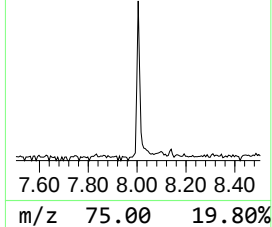
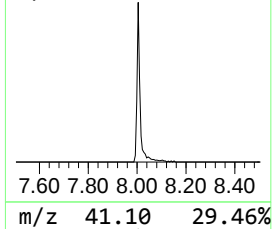
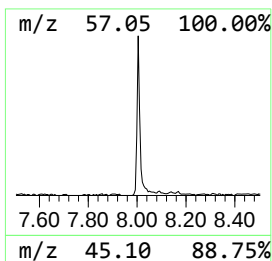
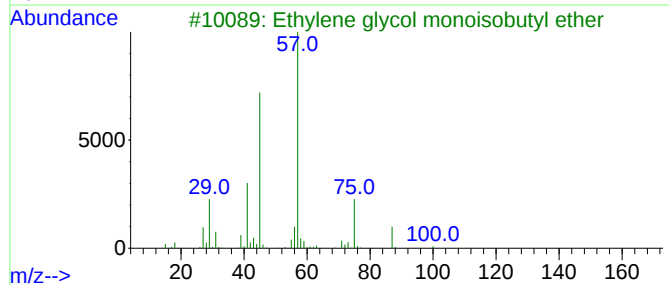
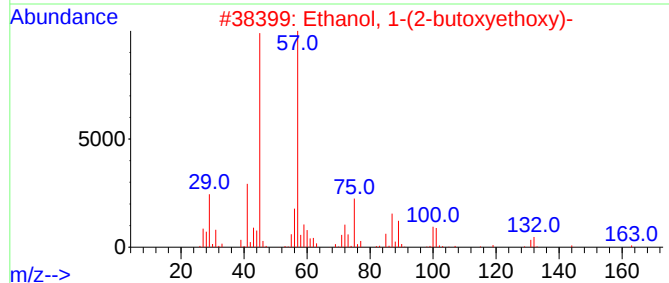
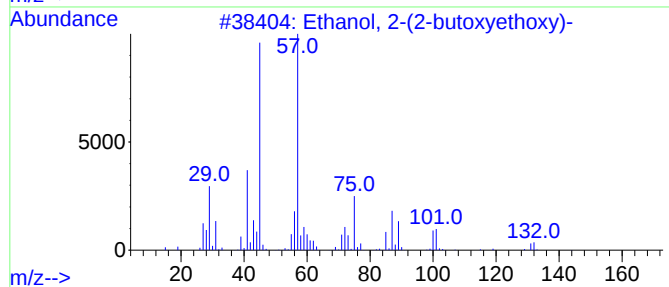
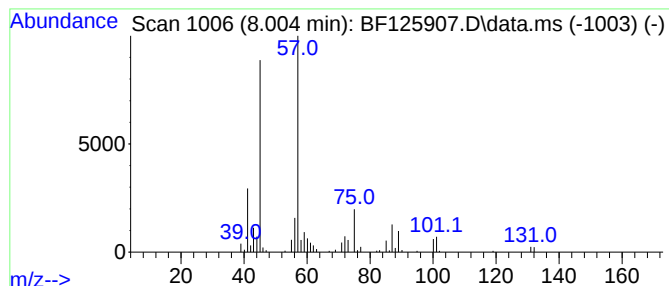
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	3.25 ng	187757	Naphthalene-d8	8.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56



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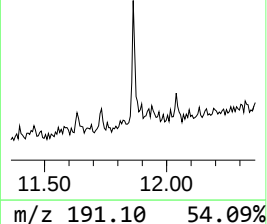
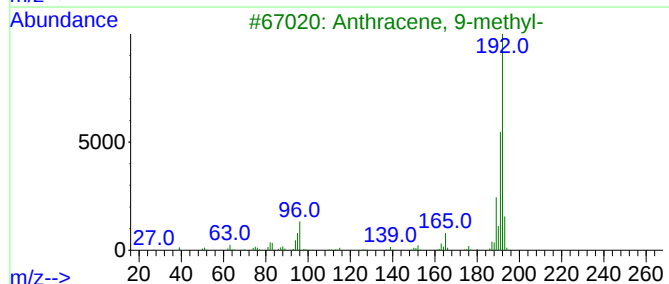
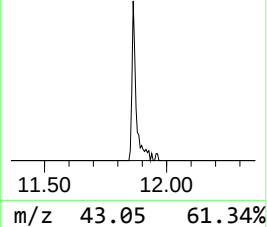
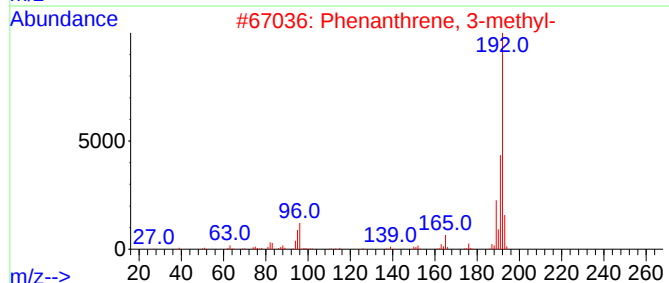
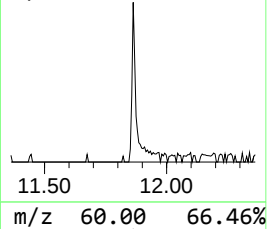
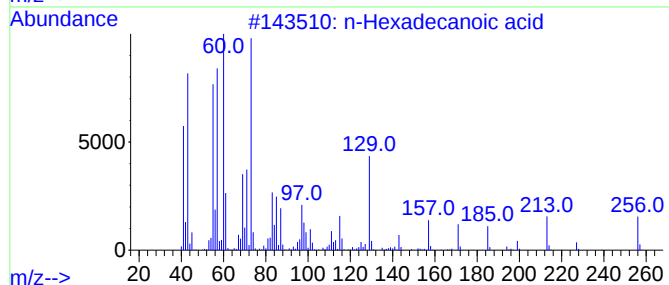
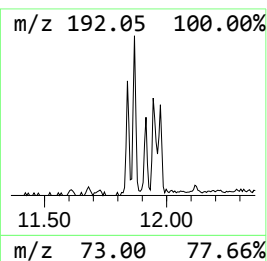
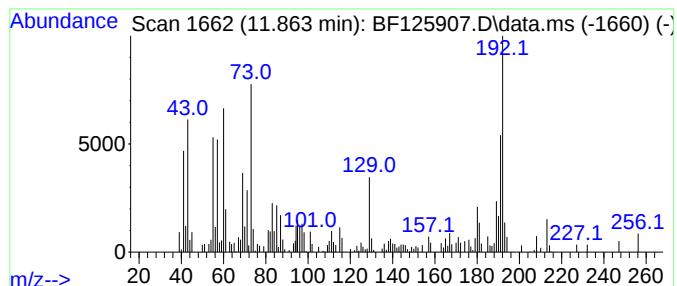
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	2.41 ng	136582	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	80
3			Anthracene, 9-methyl-	192	C15H12	000779-02-2	80
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	42



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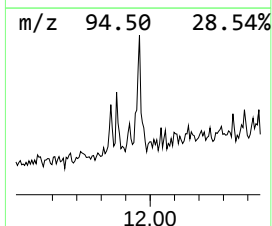
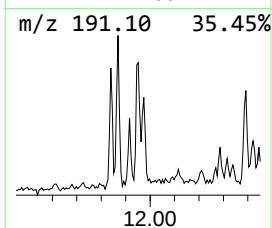
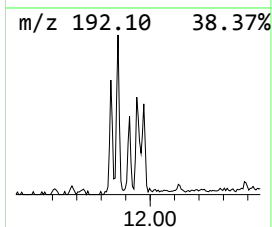
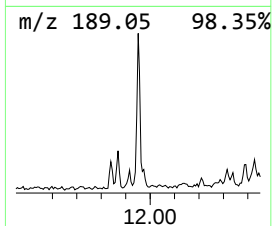
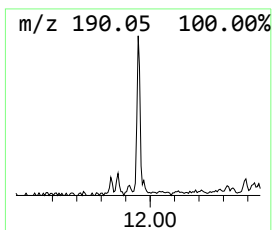
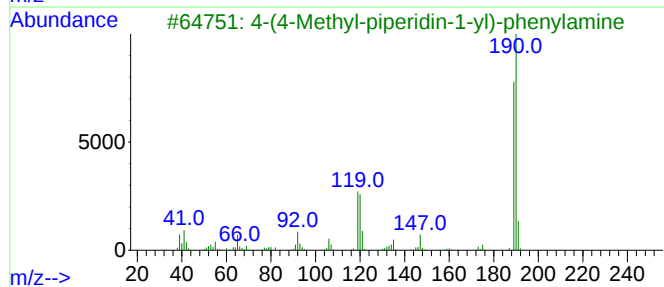
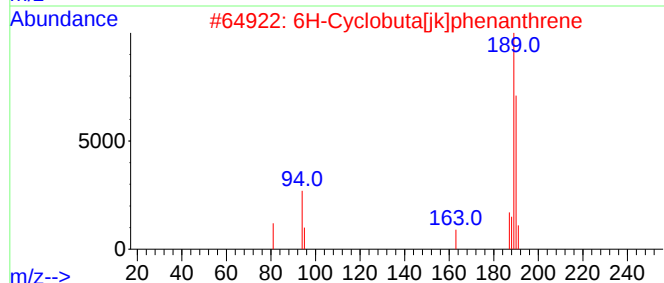
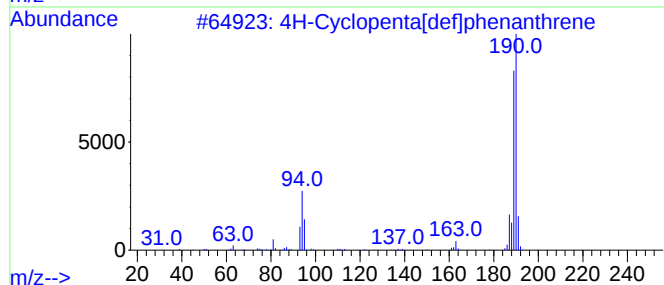
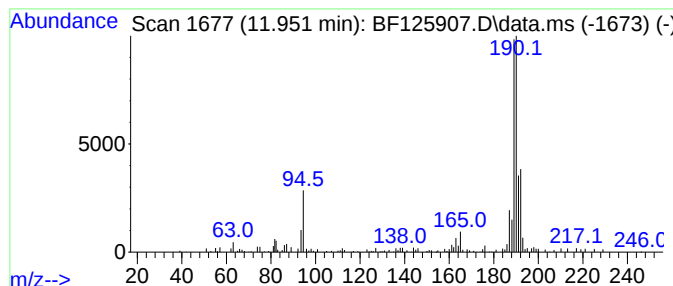
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.03 ng	115454	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3			4-(4-Methyl-piperidin-1-yl)-phen...	190	C12H18N2	342013-25-6	38
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
5			1-(Phenylethynyl)-1H-1,2,3-benzo...	219	C14H9N3	209912-23-2	27



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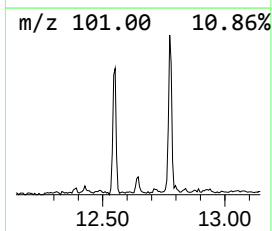
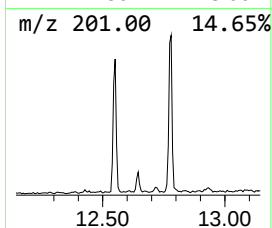
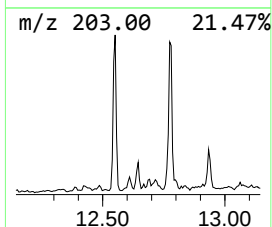
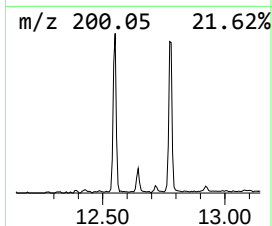
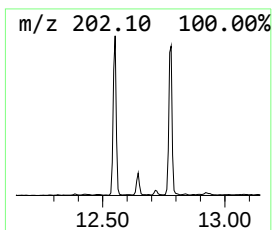
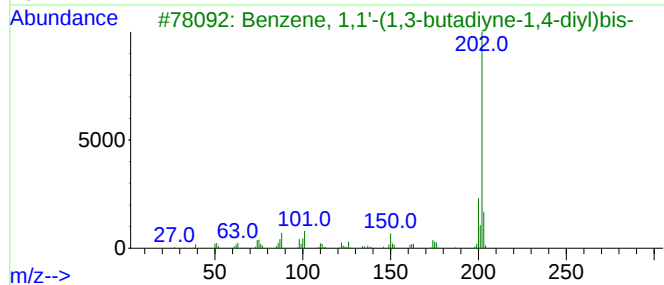
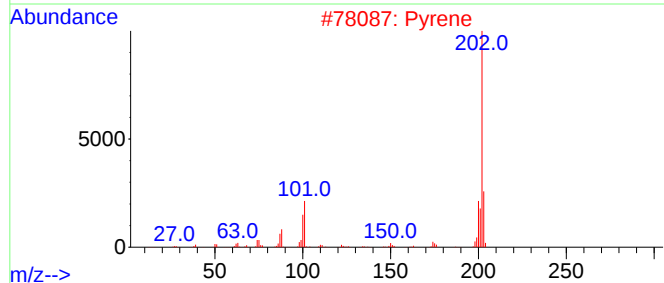
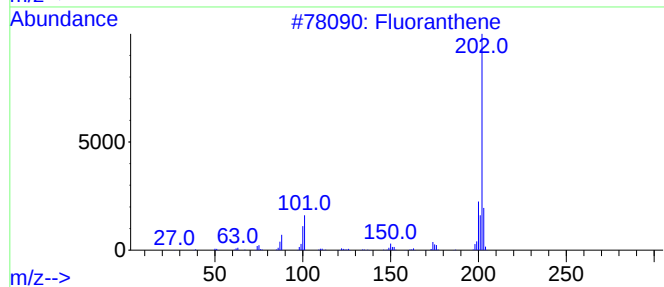
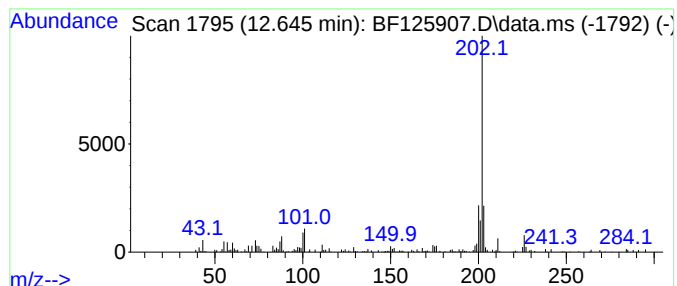
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.08 ng	118083	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene	202	C16H10	000206-44-0	94
2			Pyrene	202	C16H10	000129-00-0	83
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	60
5			7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	47



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.004	3.3	ng	187757	2	8.104	1154260	20.0
n-Hexadecanoic ...	11.863	2.4	ng	136582	4	11.339	1135190	20.0
4H-Cyclopenta[d...	11.951	2.0	ng	115454	4	11.339	1135190	20.0
Benzene, 1,1'-(...	12.645	2.1	ng	118083	4	11.339	1135190	20.0