

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010622\
 Data File : BF126524.D
 Acq On : 6 Jan 2022 18:04
 Operator : JU/CG
 Sample : N1038-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RP-RB21137

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126524.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	488	492	499	rVB	149589	179990	9.21%	0.988%
2	5.392	558	562	565	rBV	2095728	1909272	97.65%	10.477%
3	6.410	730	735	738	rBV	2004238	1955283	100.00%	10.729%
4	6.775	794	797	801	rBV	604319	542372	27.74%	2.976%
5	7.339	888	893	896	rBV	1422882	1303770	66.68%	7.154%
6	7.969	996	1000	1011	rBV	83893	89265	4.57%	0.490%
7	8.063	1011	1016	1019	rBV	780225	742236	37.96%	4.073%
8	9.139	1194	1199	1202	rBV	2188312	1946424	99.55%	10.681%
9	9.816	1310	1314	1317	rBV	918614	748861	38.30%	4.109%
10	9.845	1317	1319	1322	rVB	38444	31995	1.64%	0.176%
11	10.363	1404	1407	1412	rBV	38100	33128	1.69%	0.182%
12	10.604	1444	1448	1455	rBV	1229418	1060158	54.22%	5.817%
13	10.733	1466	1470	1477	rVB3	17268	29019	1.48%	0.159%
14	11.304	1563	1567	1569	rBV	747196	693691	35.48%	3.807%
15	11.327	1569	1571	1574	rVV	193045	154498	7.90%	0.848%
16	11.374	1576	1579	1583	rVB	136270	114421	5.85%	0.628%
17	11.833	1654	1657	1662	rBV2	43548	45232	2.31%	0.248%
18	11.916	1668	1671	1674	rBV2	48612	52685	2.69%	0.289%
19	12.104	1698	1703	1705	rBV	18548	21843	1.12%	0.120%
20	12.121	1705	1706	1712	rVB2	25504	22598	1.16%	0.124%
21	12.357	1742	1746	1748	rBV2	17508	20802	1.06%	0.114%
22	12.439	1757	1760	1765	rVB	28155	27461	1.40%	0.151%
23	12.516	1769	1773	1777	rBV	405212	338665	17.32%	1.858%
24	12.745	1806	1812	1815	rBV	337064	340415	17.41%	1.868%
25	12.792	1818	1820	1826	rVB2	20718	30597	1.56%	0.168%
26	12.863	1829	1832	1833	rBV	27331	22515	1.15%	0.124%
27	12.892	1833	1837	1840	rVV	1536221	1363168	69.72%	7.480%
28	12.963	1844	1849	1853	rBV3	29536	47356	2.42%	0.260%
29	13.074	1861	1868	1871	rVB3	69121	116075	5.94%	0.637%
30	13.139	1875	1879	1882	rBV	69088	57390	2.94%	0.315%
31	13.174	1882	1885	1888	rBV2	45098	47990	2.45%	0.263%
32	13.268	1898	1901	1904	rVB	41372	35131	1.80%	0.193%
33	13.298	1904	1906	1908	rBV	27526	25802	1.32%	0.142%
34	13.327	1908	1911	1914	rVB3	23677	24492	1.25%	0.134%
35	13.580	1952	1954	1958	rVB	30481	35245	1.80%	0.193%
36	13.692	1968	1973	1976	rBV2	37728	50792	2.60%	0.279%

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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-BF122921.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.810	1987	1993	2000	rVB4	36969	77755	3.98%	0.427%
38	13.945	2009	2016	2018	rBV2	605075	751288	38.42%	4.123%
39	13.968	2018	2020	2023	rVB	237379	188198	9.63%	1.033%
40	14.045	2029	2033	2039	rBV2	77626	111454	5.70%	0.612%
41	14.157	2050	2052	2057	rVB2	23819	25997	1.33%	0.143%
42	14.333	2077	2082	2085	rVB2	45344	51455	2.63%	0.282%
43	14.368	2085	2088	2092	rVB2	38460	38943	1.99%	0.214%
44	14.427	2092	2098	2100	rBV4	31489	45228	2.31%	0.248%
45	14.457	2100	2103	2105	rVV4	45123	47027	2.41%	0.258%
46	14.480	2105	2107	2111	rVV4	26673	31901	1.63%	0.175%
47	14.533	2111	2116	2122	rVB6	18943	32794	1.68%	0.180%
48	14.639	2130	2134	2137	rBV5	19396	27350	1.40%	0.150%
49	14.804	2159	2162	2168	rBV2	50011	74648	3.82%	0.410%
50	14.886	2172	2176	2179	rVB3	20746	31420	1.61%	0.172%
51	14.974	2187	2191	2194	rBV	329177	453517	23.19%	2.489%
52	15.057	2202	2205	2207	rBV2	19442	26172	1.34%	0.144%
53	15.080	2207	2209	2212	rVB	48795	42427	2.17%	0.233%
54	15.168	2220	2224	2229	rVB4	14701	26703	1.37%	0.147%
55	15.268	2236	2241	2247	rVB	216646	268496	13.73%	1.473%
56	15.327	2247	2251	2257	rBV	232348	281386	14.39%	1.544%
57	15.392	2257	2262	2265	rVV	467689	561808	28.73%	3.083%
58	15.421	2265	2267	2274	rVB2	73626	103170	5.28%	0.566%
59	15.557	2283	2290	2293	rBV5	20176	46543	2.38%	0.255%
60	15.739	2318	2321	2328	rVB4	17932	27913	1.43%	0.153%
61	15.857	2337	2341	2346	rBV2	25804	35314	1.81%	0.194%
62	16.627	2465	2472	2475	rBV4	26619	55250	2.83%	0.303%
63	16.804	2497	2502	2512	rVB2	108219	220571	11.28%	1.210%
64	16.986	2528	2533	2537	rBV3	15419	25776	1.32%	0.141%
65	17.033	2537	2541	2546	rVV2	17208	29090	1.49%	0.160%
66	17.233	2569	2575	2586	rVB2	86737	179959	9.20%	0.987%
67	17.392	2595	2602	2604	rBV6	11419	22044	1.13%	0.121%
68	17.462	2610	2614	2619	rVB5	11240	21599	1.10%	0.119%

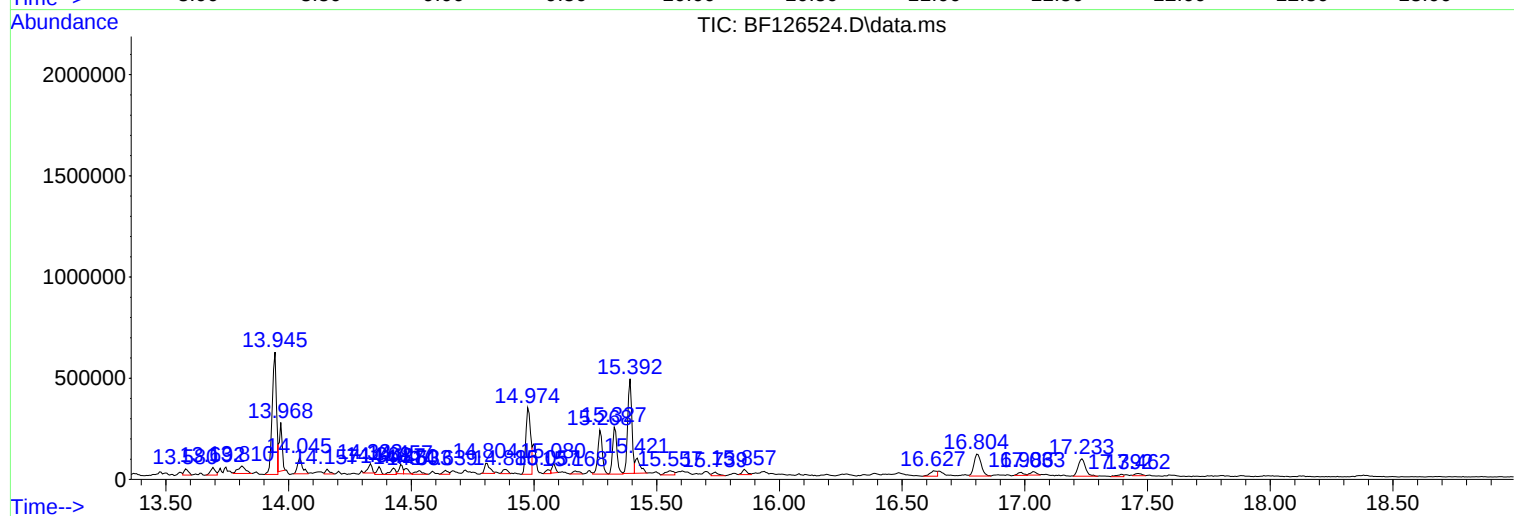
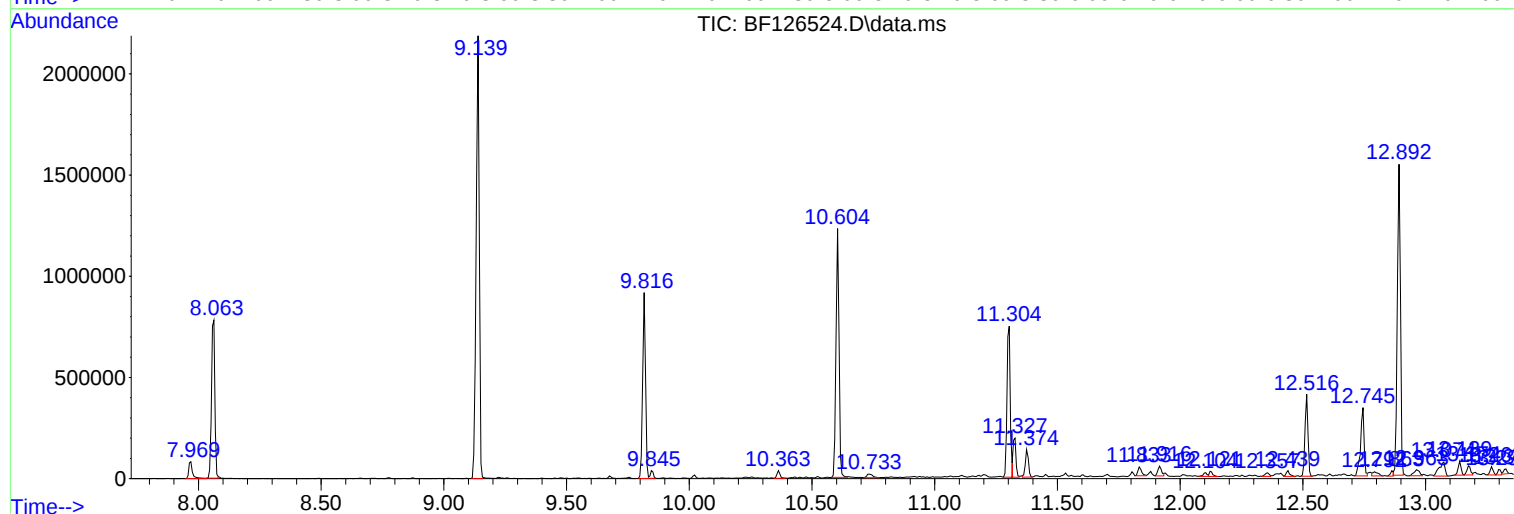
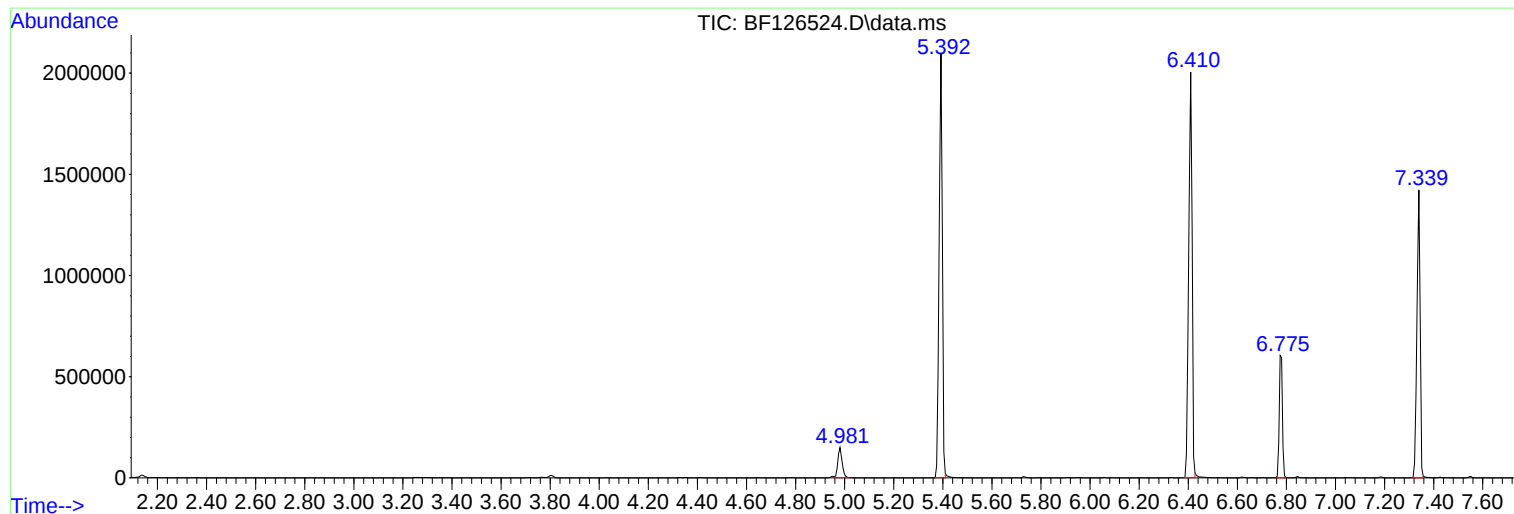
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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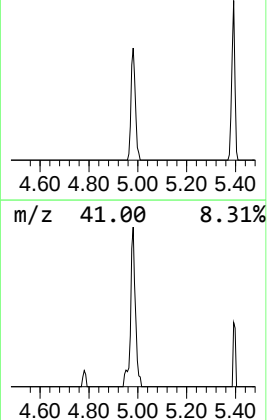
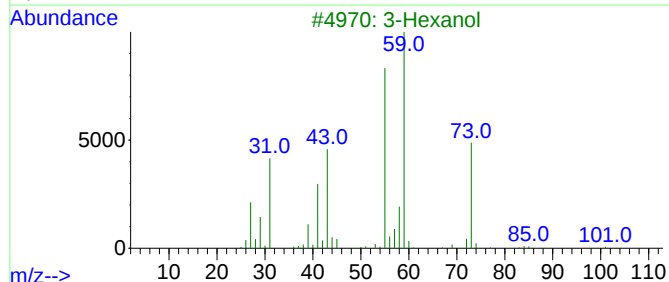
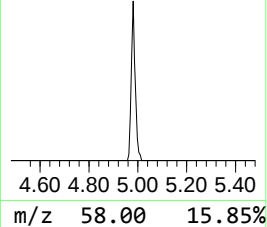
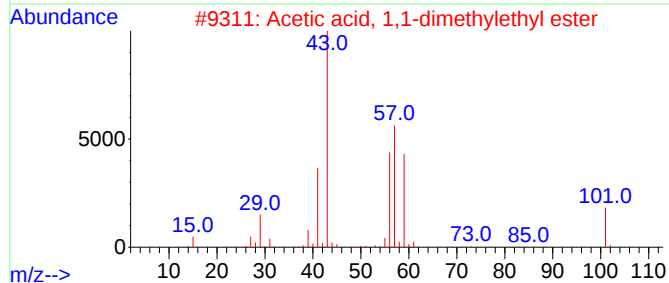
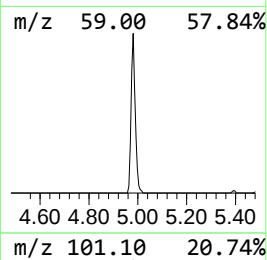
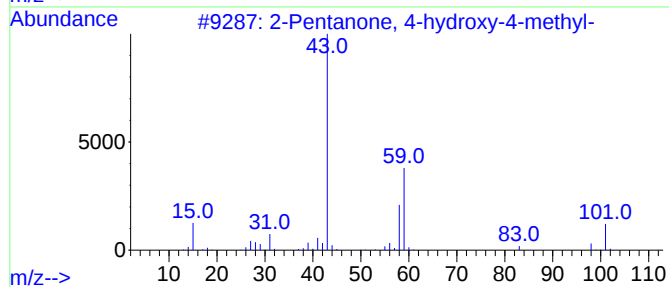
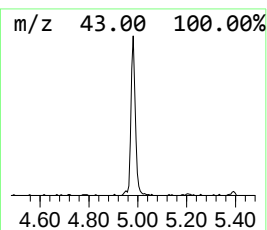
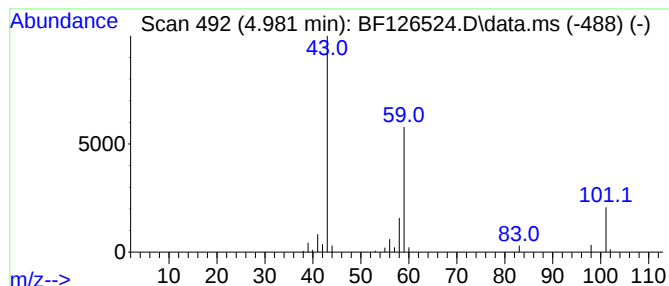
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
4.981	6.64 ng	179990	1,4-Dichlorobenzene-d4	6.781	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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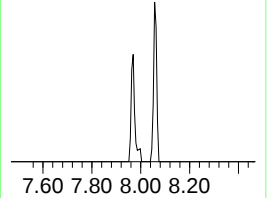
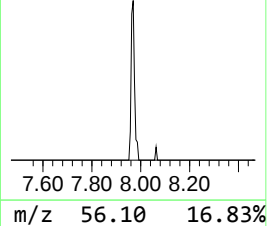
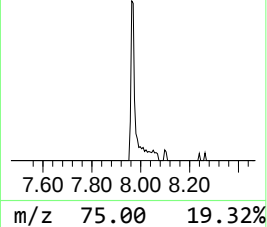
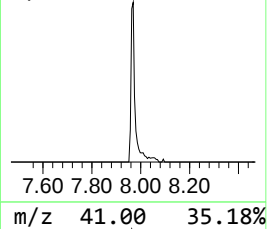
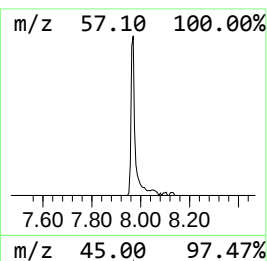
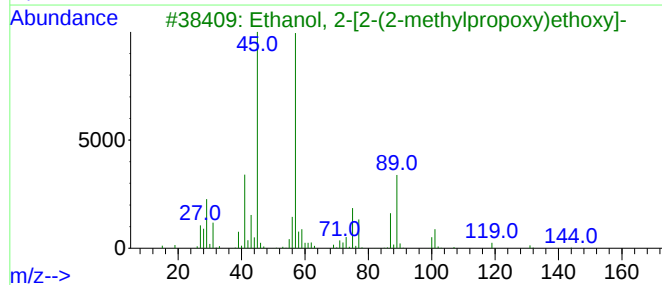
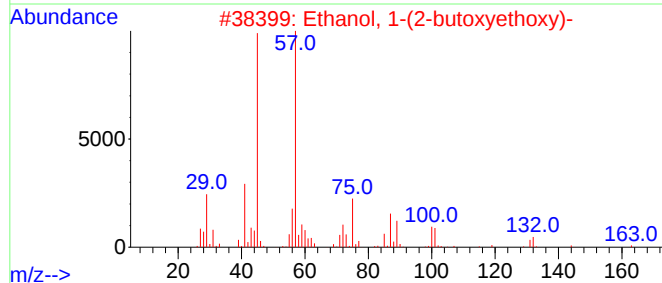
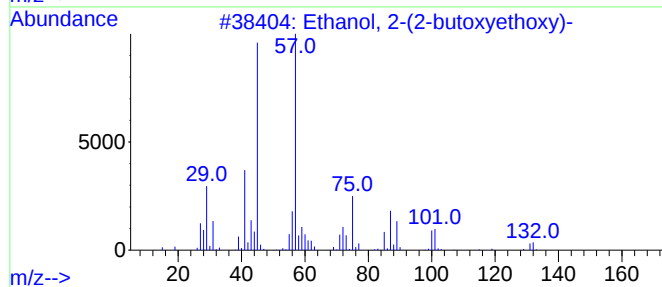
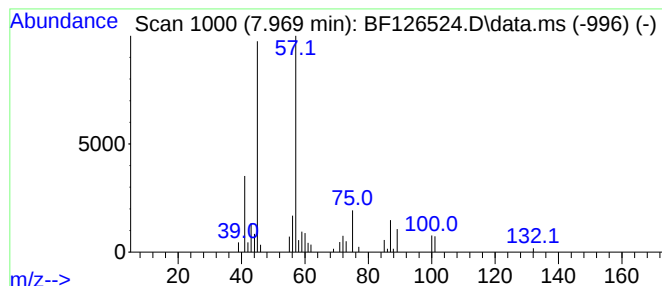
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	2.41 ng	89265	Naphthalene-d8	8.063

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	90
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	56
4			Hexane, 1-(methoxymethoxy)-	146	C8H18O2	066675-06-7	50
5			Propanoic acid, 3-methoxy-2-methoxy-	132	C6H12O3	003852-11-7	50



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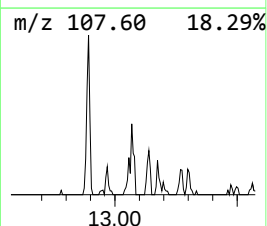
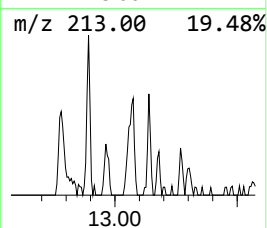
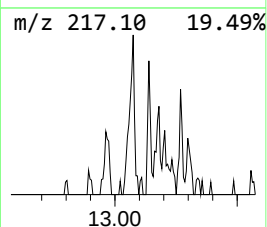
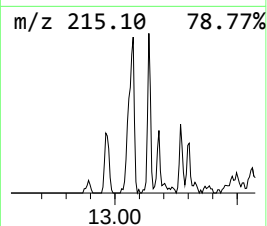
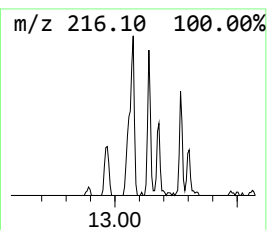
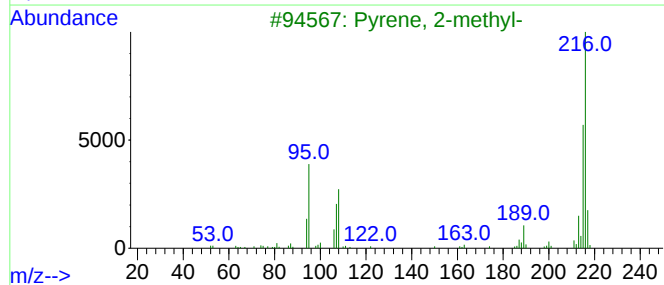
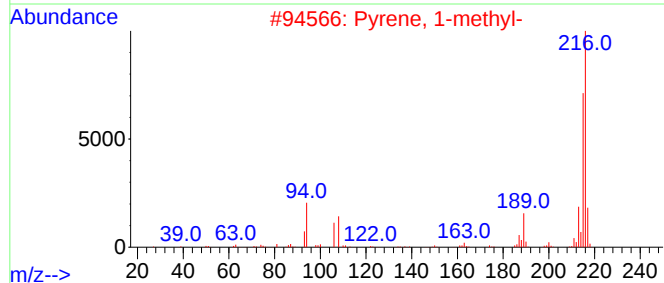
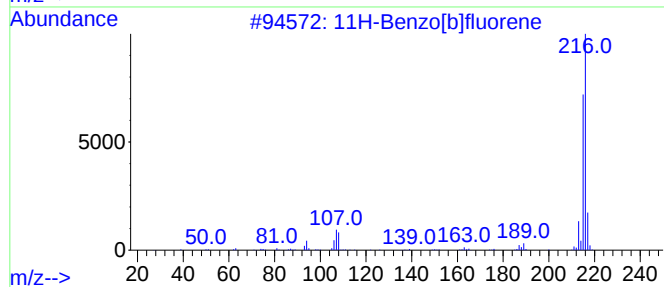
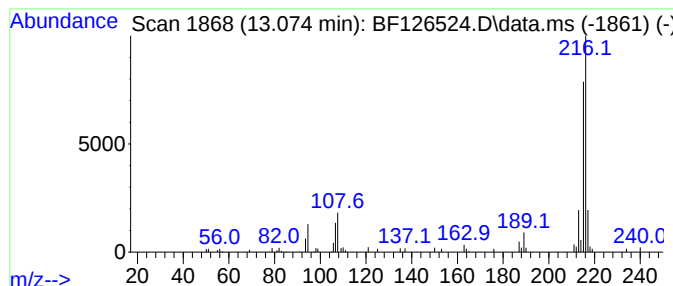
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 11H-Benzo[b]fluorene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.074	3.09 ng	116075	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
3			Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
5			Fluoranthene, 2-methyl-	216	C17H12	003543-31-6	87



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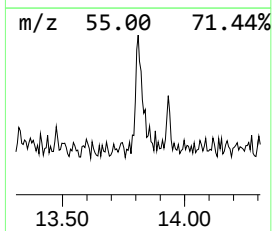
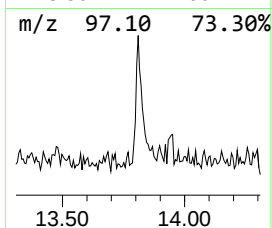
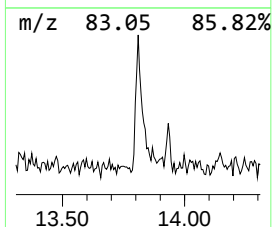
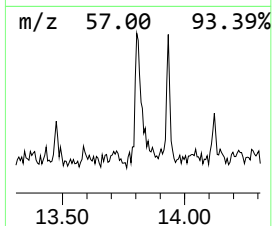
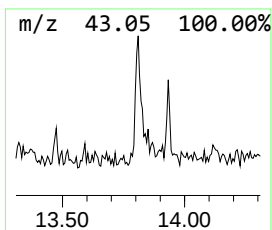
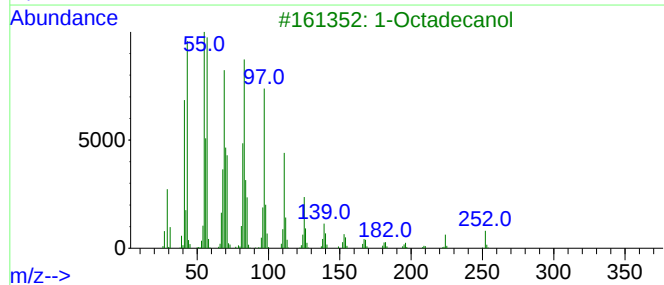
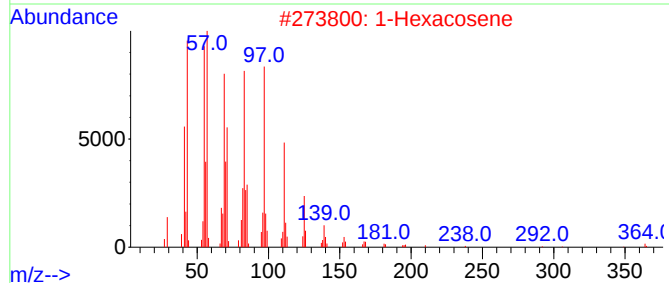
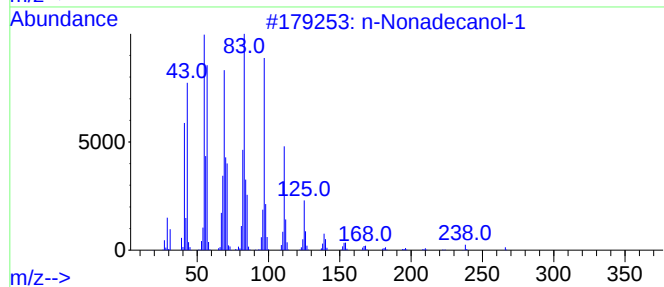
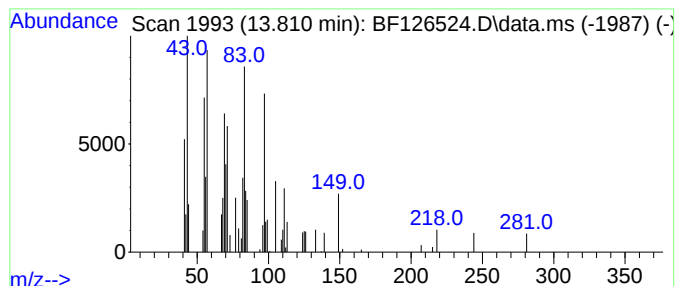
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Nonadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.810	2.07 ng	77755	Chrysene-d12	13.945	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	83
2	1-Hexacosene	364	C26H52	018835-33-1	83
3	1-Octadecanol	270	C18H38O	000112-92-5	81
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	72
5	Isoheptadecanol	256	C17H36O	057289-07-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010622\
Data File : BF126524.D
Acq On : 6 Jan 2022 18:04
Operator : JU/CG
Sample : N1038-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RP-RB21137

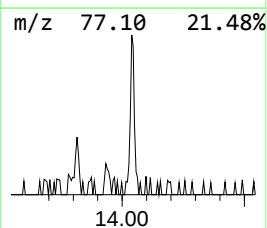
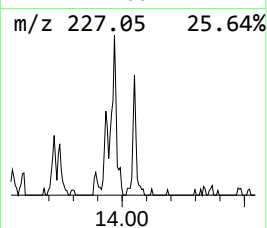
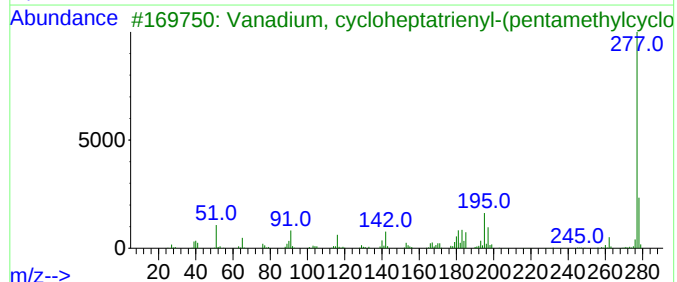
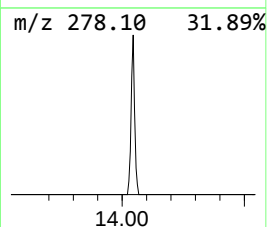
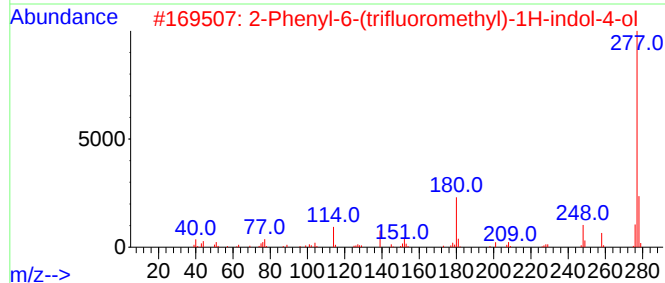
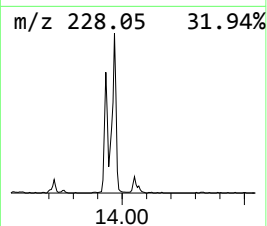
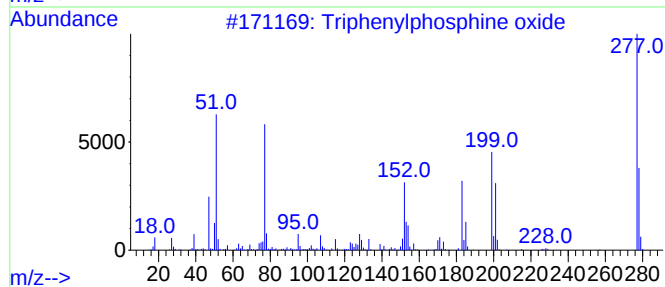
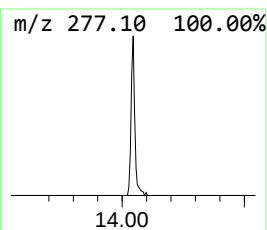
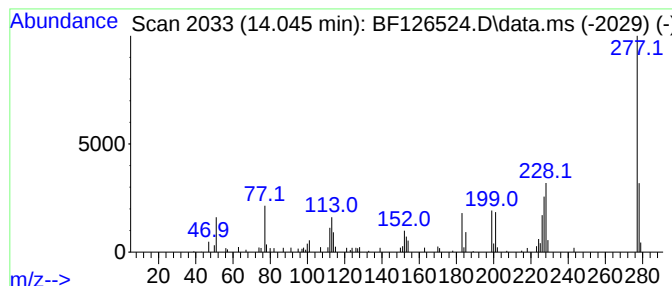
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.045 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.045	2.97 ng	111454	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	46
2			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	43
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35
5			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010622\
Data File : BF126524.D
Acq On : 6 Jan 2022 18:04
Operator : JU/CG
Sample : N1038-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RP-RB21137

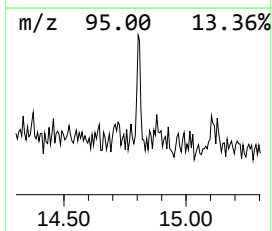
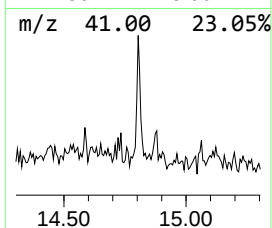
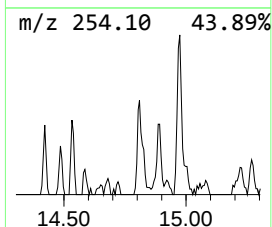
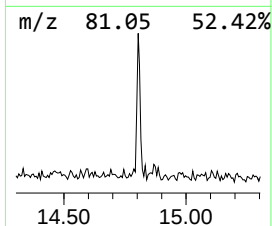
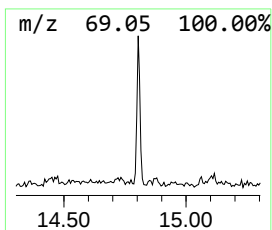
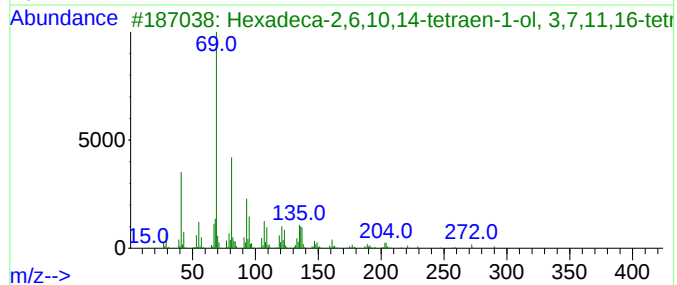
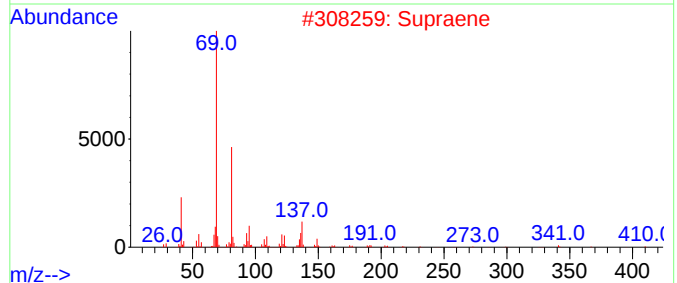
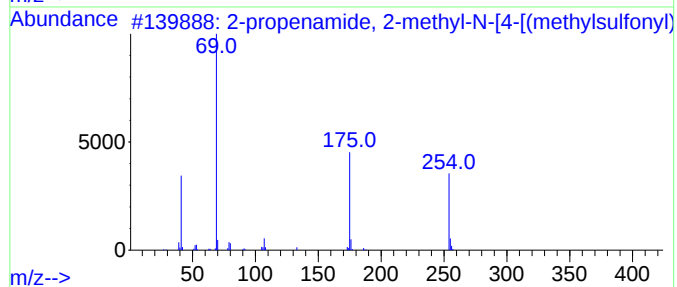
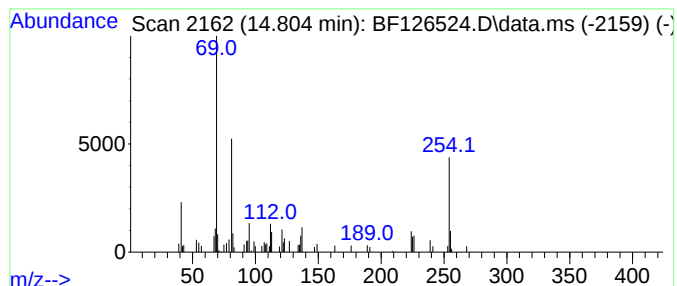
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-propenamide, 2-methyl-N-[... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.66 ng	74648	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-propenamide, 2-methyl-N-[4-[(m...	254	C11H14N2O3S	1000401-43-5	50
2			Supraene	410	C30H50	007683-64-9	46
3			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	37
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	37
5			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010622\
Data File : BF126524.D
Acq On : 6 Jan 2022 18:04
Operator : JU/CG
Sample : N1038-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RP-RB21137

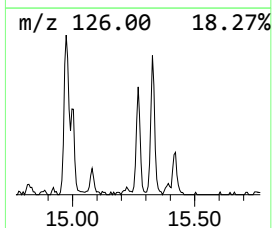
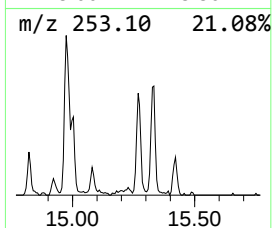
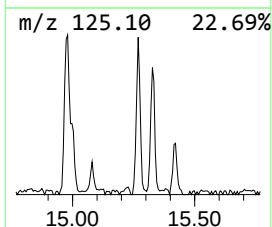
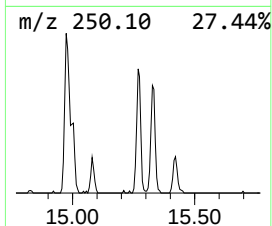
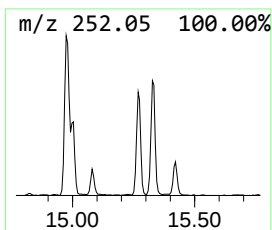
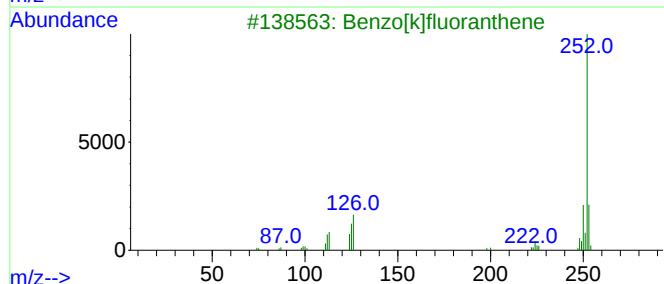
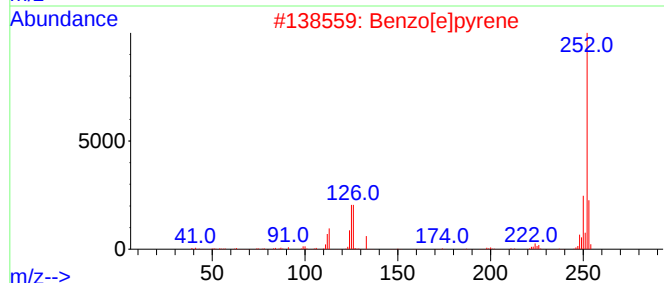
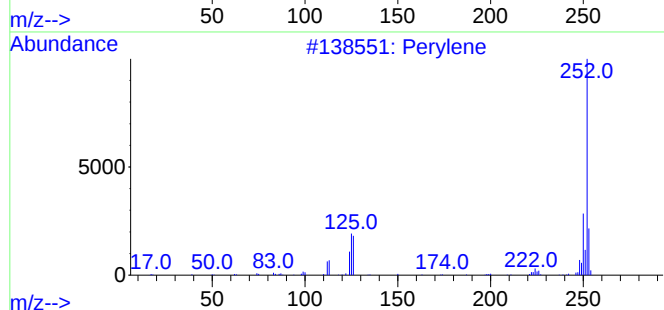
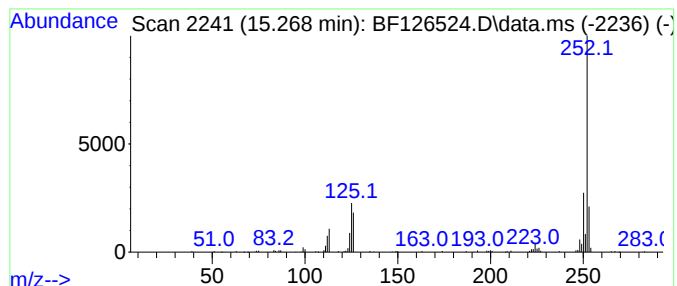
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.268	9.56 ng	268496	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010622\
Data File : BF126524.D
Acq On : 6 Jan 2022 18:04
Operator : JU/CG
Sample : N1038-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RP-RB21137

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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-...	4.981	6.6	ng	179990	1	6.781	542372	20.0
Ethanol, 2-(2-b...	7.969	2.4	ng	89265	2	8.063	742236	20.0
11H-Benzo[b]flu...	13.074	3.1	ng	116075	5	13.945	751288	20.0
n-Nonadecanol-1	13.810	2.1	ng	77755	5	13.945	751288	20.0
unknown14.045	14.045	3.0	ng	111454	5	13.945	751288	20.0
2-propenamide, ...	14.804	2.7	ng	74648	6	15.392	561808	20.0
Perylene	15.268	9.6	ng	268496	6	15.392	561808	20.0