LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

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-BF062922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129112.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.198	492	495	506	rVB	50149	66734	1.37%	0.122%
2	5.575	555	559	563	rBV	4212521	4000494	82.17%	7.328%
3	6.575	724	729	732	rBV	4393066	3919360	80.50%	7.179%
4	6.598	732	733	743	rVB	99686	109052	2.24%	0.200%
5	6.957	790	794	797	rBV	2840699	2191094	45.00%	4.013%
6	7.516	885	889	892	rBV	3095499	2524606	51.85%	4.624%
7	8.239	1008	1012	1015	rBV	3590345	2811917	57.76%	5.151%
8	9.051	1147	1150	1153	rVB	68887	58569	1.20%	0.107%
9	9.251	1182	1184	1186	rVB	134370	88254	1.81%	0.162%
10	9.316	1191	1195	1198	rBV	5705232	4868638	100.00%	8.918%
11	9.386	1204	1207	1211	rBV2	252183	264522	5.43%	0.485%
12	9.581	1236	1240	1245	rBV3	87927	137881	2.83%	0.253%
13	9.651	1249	1252	1255	rVV2	90118	104454	2.15%	0.191%
14	9.704	1258	1261	1264	rVV	444724	353467	7.26%	0.647%
15	9.769	1269	1272	1274	rBV3	79266	81339	1.67%	0.149%
16	9.863	1284	1288	1290	rBV	189634	187229	3.85%	0.343%
17	9.916	1293	1297	1299	rVB2	227015	248043	5.09%	0.454%
18	9.998	1308	1311	1314	rVB	3493025	2762899	56.75%	5.061%
19	10.028	1314	1316	1325	rVB2	174756	246891	5.07%	0.452%
20	10.204	1343	1346	1348	rVB2	137045	120224	2.47%	0.220%
21	10.239	1349	1352	1356	rVB2	124145	126655	2.60%	0.232%
22	10.316	1362	1365	1367	rBV3	91215	95607	1.96%	0.175%
23	10.416	1378	1382	1385	rVB3	216630	229964	4.72%	0.421%
24	10.545	1401	1404	1411	rVB	304904	315219	6.47%	0.577%
25	10.639	1417	1420	1422	rVB2	217808	203756	4.19%	0.373%
26	10.704	1426	1431	1435	rBV4	110405	164741	3.38%	0.302%
27	10.786	1442	1445	1450	rBV	2831517	2517485	51.71%	4.611%
28	10.904	1460	1465	1469	rBV2	636107	747130	15.35%	1.369%
29	10.986	1476	1479	1481	rBV	99699	82585	1.70%	0.151%
30	11.010	1481	1483	1488	rBV3	51123	61999	1.27%	0.114%
31	11.292	1529	1531	1536	rBV	116175	108675	2.23%	0.199%
32	11.339	1536	1539	1541	rBV2	230008	182995	3.76%	0.335%
33	11.369	1541	1544	1546	rBV	224492	234930	4.83%	0.430%
34	11.492	1561	1565	1567	rBV	2999119	2630208	54.02%	4.818%
35	11.516	1567	1569	1573	rVV	2608490	2032825	41.75%	3.723%
36	11.569	1575	1578	1580	rVV	404234	313940	6.45%	0.575%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

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-BF062922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.722	1601	1604	1609	rBV2	144969	139797	2.87%	0.256%
38	11.769	1609	1612	1614	rBV	192782	129328	2.66%	0.237%
39	11.869	1627	1629	1632	rVB	127234	117593	2.42%	0.215%
40	11.998	1648	1651	1653	rBV2	364919	435632	8.95%	0.798%
41	12.022	1653	1655	1659	rVB	384983	318977	6.55%	0.584%
42	12.069	1661	1663	1666	rBV	91879	73961	1.52%	0.135%
43	12.110	1666	1670	1672	rBV2	357466	361018	7.42%	0.661%
44	12.180	1679	1682	1684	rBV	139351	131102	2.69%	0.240%
45	12.292	1698	1701	1703	rBV	175627	158942	3.26%	0.291%
46	12.316	1703	1705	1708	rVB	127261	101086	2.08%	0.185%
47	12.545	1741	1744	1746	rBV	107169	95842	1.97%	0.176%
48	12.580	1746	1750	1753	rVV3	251365	300274	6.17%	0.550%
49	12.633	1756	1759	1763	rBV2	104558	123063	2.53%	0.225%
50	12.710	1768	1772	1776	rBV	2791075	2258135	46.38%	4.136%
51	12.939	1805	1811	1814	rBV	2017606	2301566	47.27%	4.216%
52	12.969	1814	1816	1824	rVB2	539009	1010781	20.76%	1.851%
53	13.080	1831	1835	1838	rVB	4496951	3639222	74.75%	6.666%
54	13.268	1864	1867	1870	rVB	282326	248629	5.11%	0.455%
55	13.333	1876	1878	1881	rVB2	177393	148775	3.06%	0.273%
56	13.374	1882	1885	1888	rVB2	158916	163330	3.35%	0.299%
57	14.145	2011	2016	2018	rBV2	2327659	2877253	59.10%	5.270%
58	14.168	2018	2020	2026	rVB	816438	689879	14.17%	1.264%
59	14.239	2029	2032	2036	rVB2	366728	429687	8.83%	0.787%
60	15.215	2194	2198	2201	rBV	530529	841373	17.28%	1.541%
61	15.604	2261	2264	2270	rVB	437163	522516	10.73%	0.957%
62	15.674	2271	2276	2280	rBV	1341501	1782562	36.61%	3.265%

Sum of corrected areas: 54594704

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
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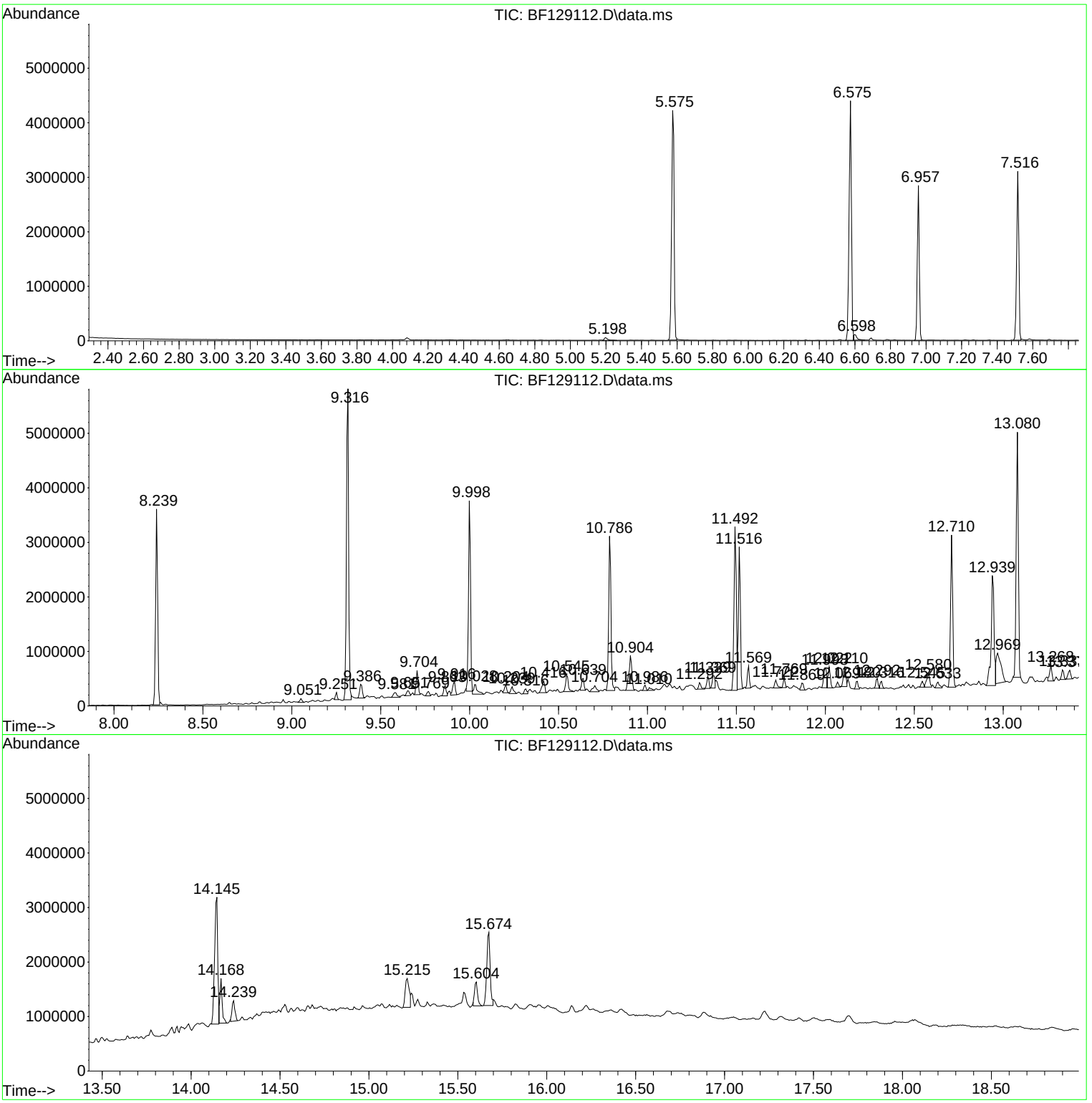
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

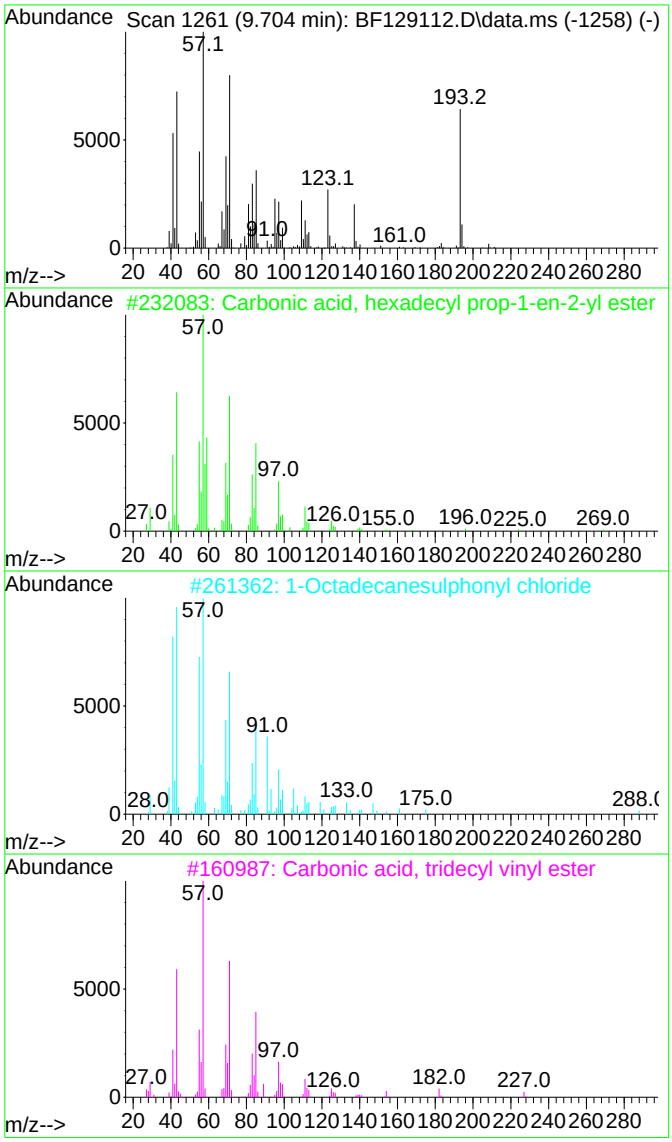
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

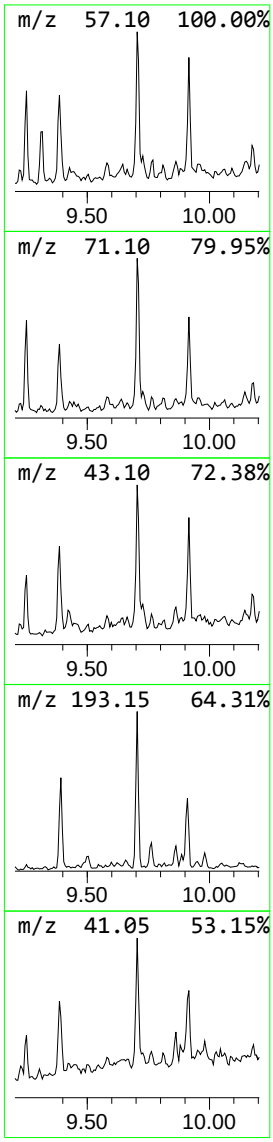
****

Peak Number 1 unknown9.704 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.704	2.56 ng	353467	Acenaphthene-d10	9.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	45
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	43
3	Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	38
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	38
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

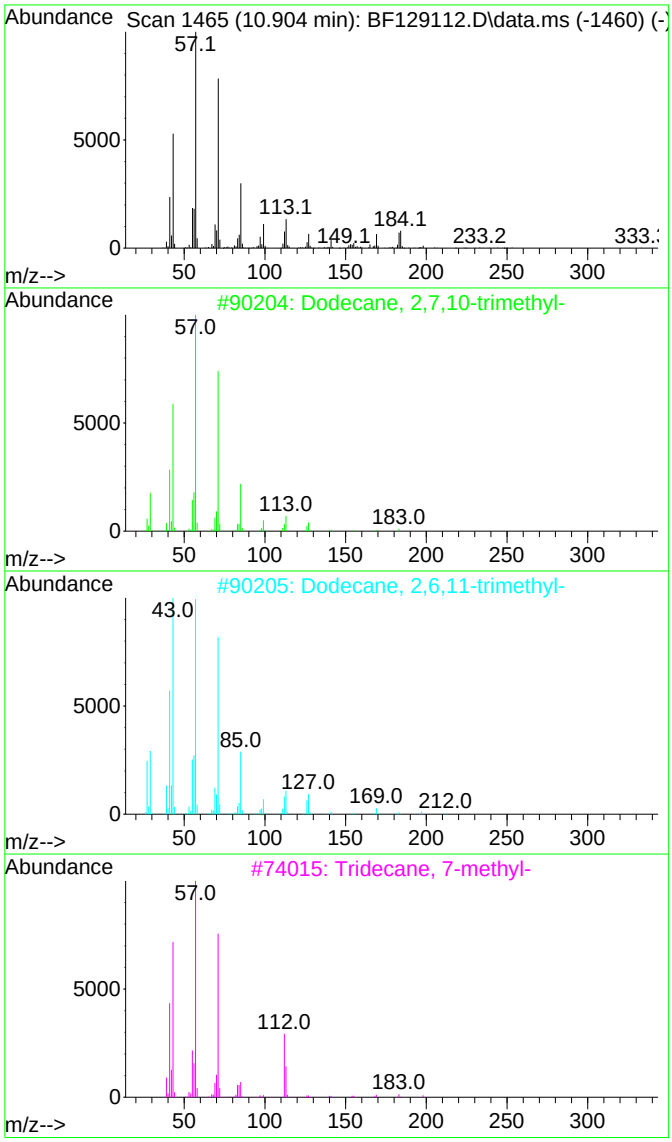
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

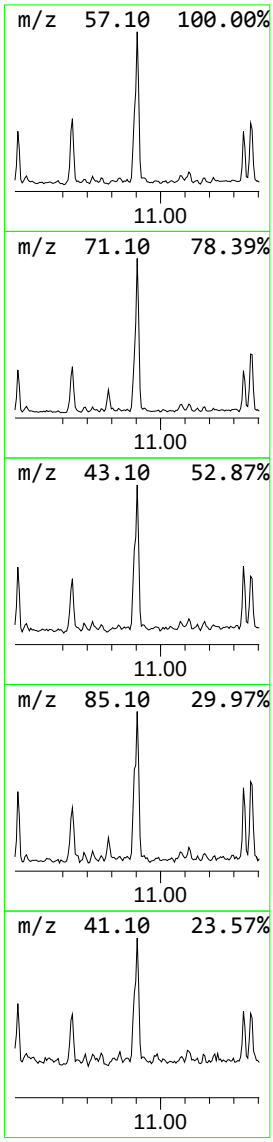
****

Peak Number 3 Dodecane, 2,7,10-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.904	5.68 ng	747130	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80
3	Tridecane, 7-methyl-	198	C14H30	026730-14-3	76
4	Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	72
5	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

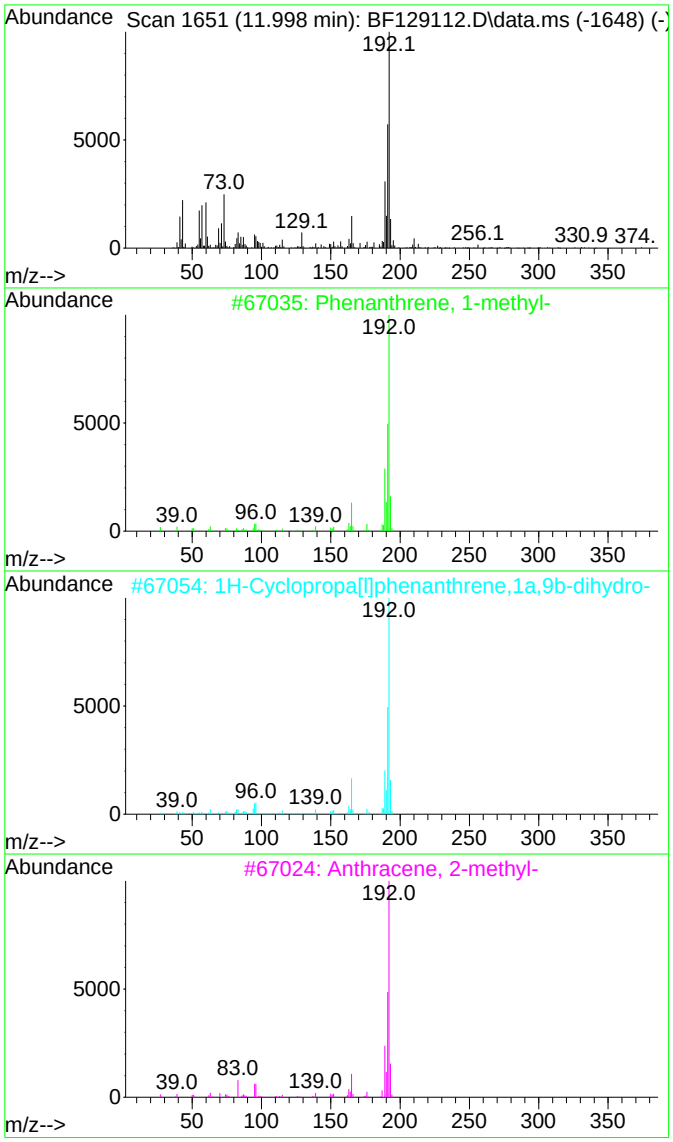
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

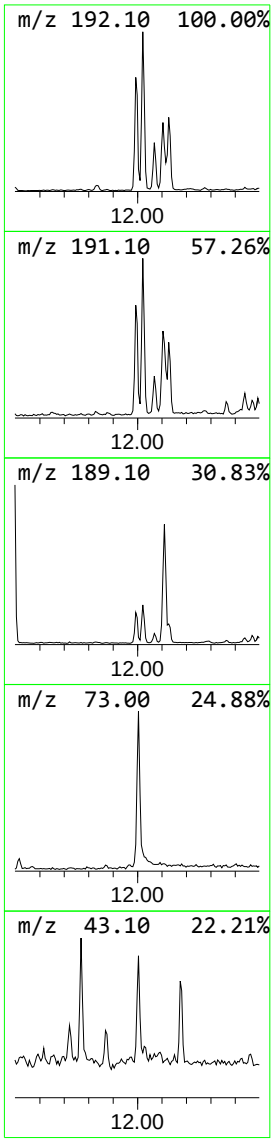
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	3.31 ng	435632	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

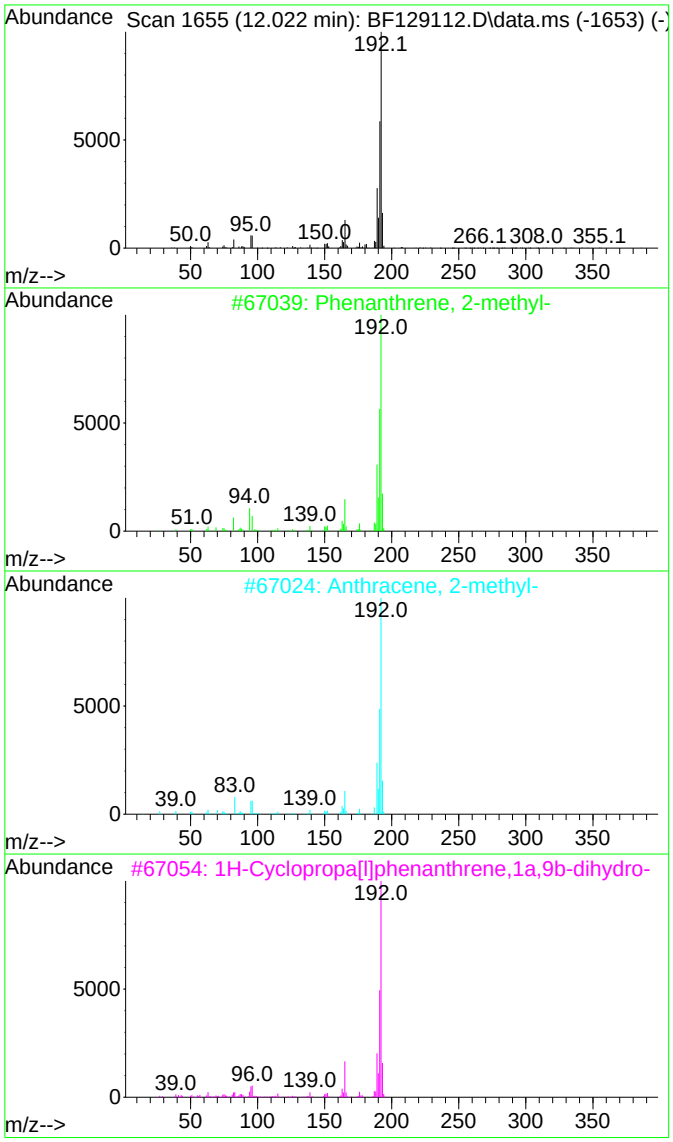
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

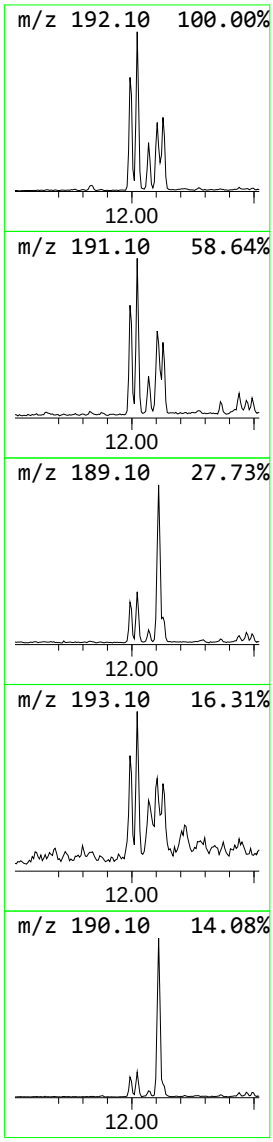
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	2.43 ng	318977	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

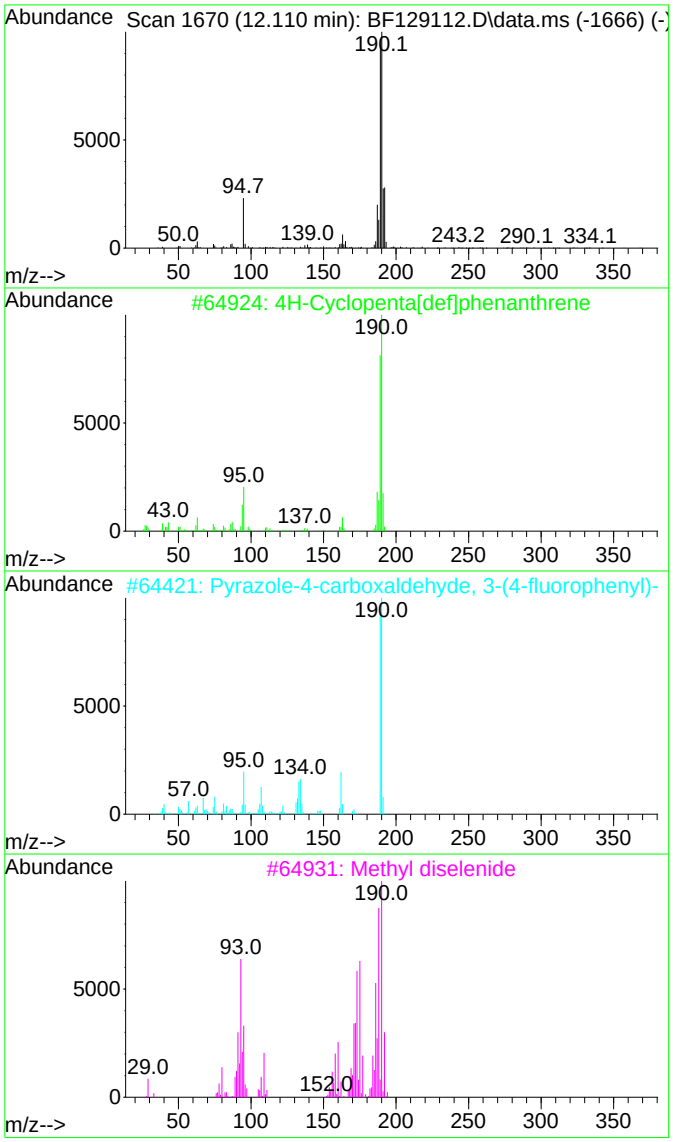
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

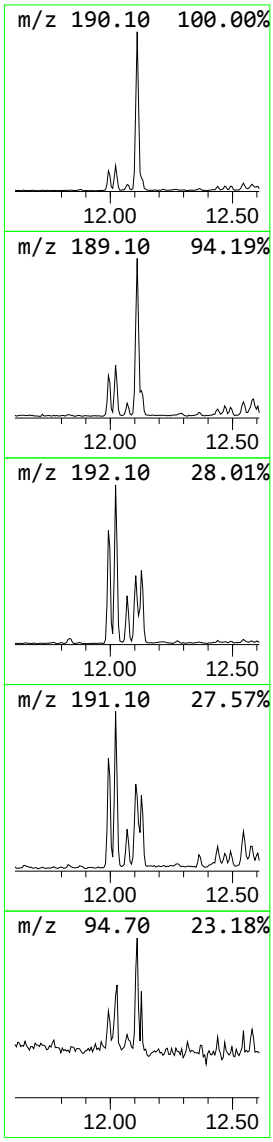
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	2.75 ng	361018	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

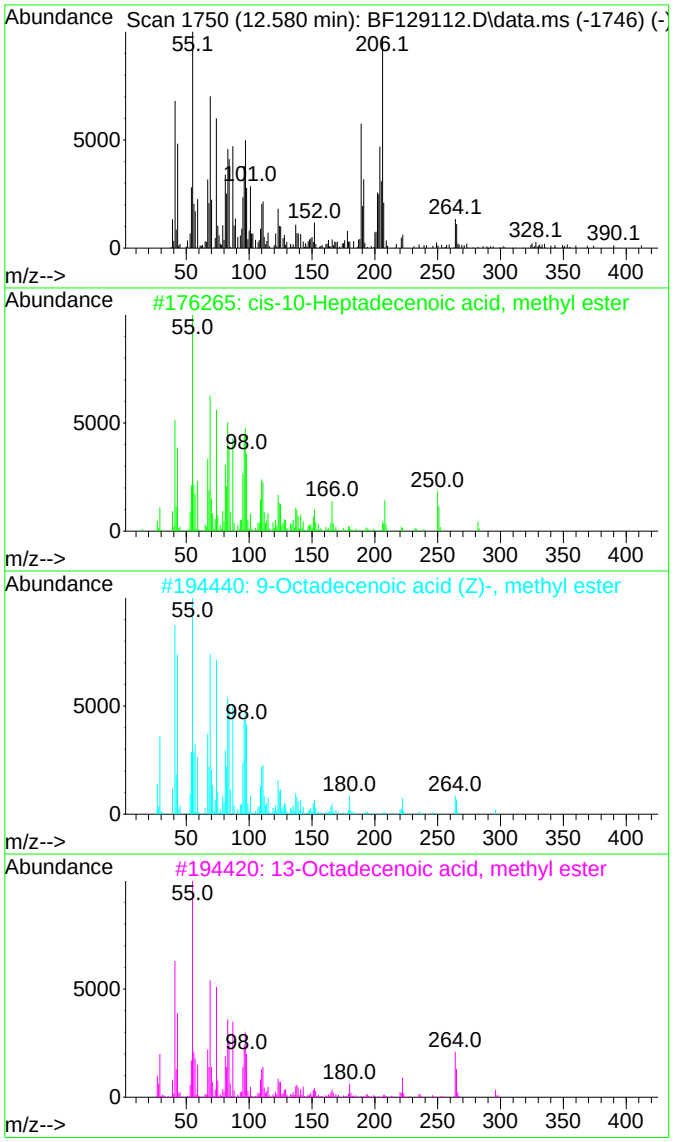
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

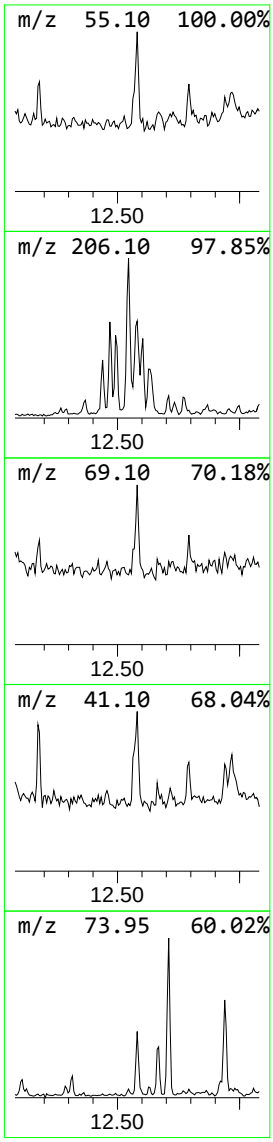
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 cis-10-Heptadecenoic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	2.28 ng	300274	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	74
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	56
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	42
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	42
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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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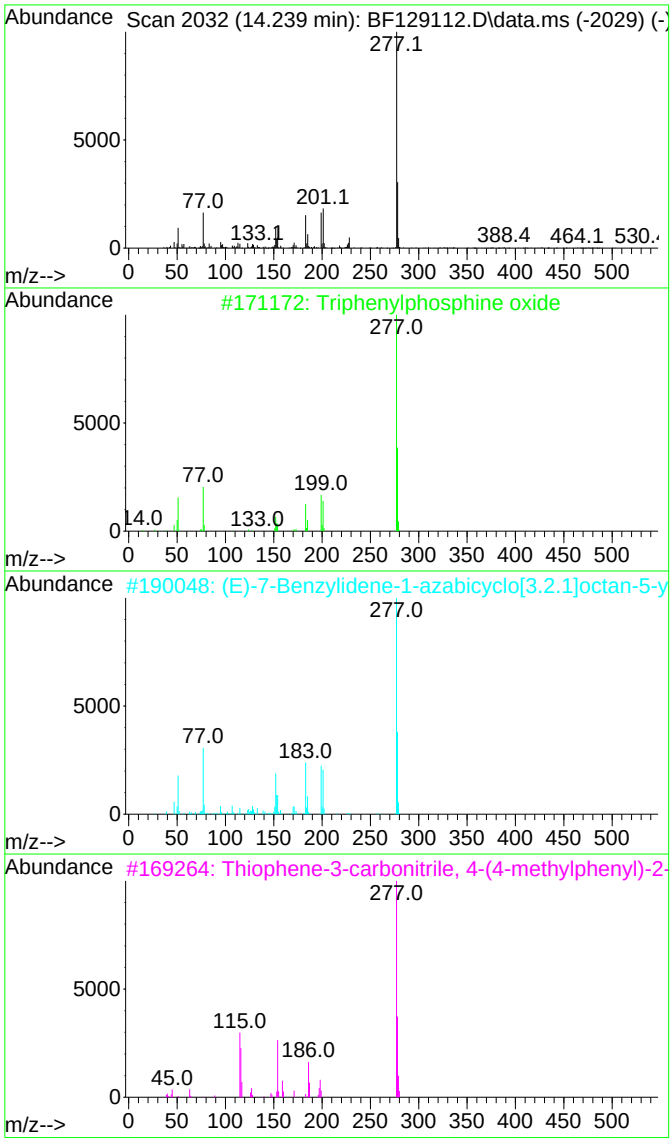
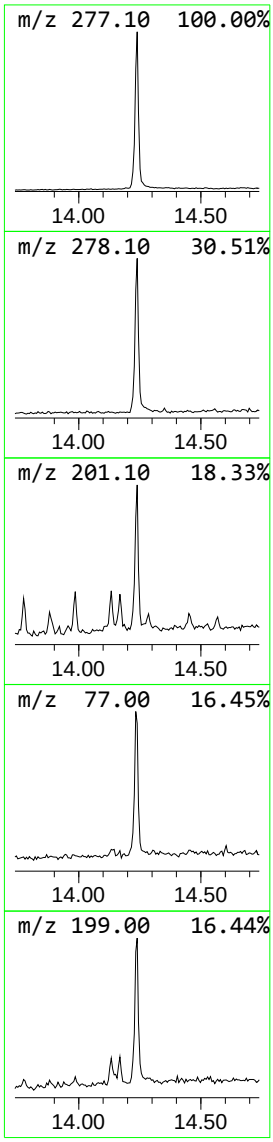
Peak Number 8 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.239	2.99 ng	429687	Chrysene-d12	14.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	86
3	Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	40
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129112.D
Acq On : 02 Jul 2022 01:30
Operator : CG\JU
Sample : N3562-11 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown9.704	9.704	2.6	ng	353467	3	9.998	2762900	20.0
Dodecane, 2,7,1...	10.904	5.7	ng	747130	4	11.492	2630210	20.0
Phenanthrene, 1...	11.998	3.3	ng	435632	4	11.492	2630210	20.0
Phenanthrene, 2...	12.022	2.4	ng	318977	4	11.492	2630210	20.0
4H-Cyclopenta[d...	12.110	2.8	ng	361018	4	11.492	2630210	20.0
cis-10-Heptadec...	12.580	2.3	ng	300274	4	11.492	2630210	20.0
Triphenylphosph...	14.239	3.0	ng	429687	5	14.145	2877250	20.0