LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	15	rVB	113678	142291	3.40%	0.403%
2	5.040	498	502	509	rVB	85756	113178	2.70%	0.321%
3	5.434	564	569	572	rBV	3657300	3714913	88.72%	10.524%
4	6.445	735	741	744	rBV	3451286	3906262	93.29%	11.066%
5	6.816	800	804	807	rBV	1377096	1141157	27.25%	3.233%
6	7.375	894	899	902	rBV	2494782	2675967	63.91%	7.581%
7	8.098	1017	1022	1039	rVB	1787291	1659210	39.63%	4.700%
8	9.175	1200	1205	1216	rBV	3856475	4187064	100.00%	11.862%
9	9.263	1216	1220	1227	rVB2	74281	94383	2.25%	0.267%
10	9.469	1253	1255	1261	rVB	67945	65850	1.57%	0.187%
11	9.792	1306	1310	1314	rVB2	43694	44595	1.07%	0.126%
12	9.851	1315	1320	1330	rBV	1844697	1761210	42.06%	4.989%
13	9.980	1337	1342	1352	rBV	1641677	1711898	40.89%	4.850%
14	10.263	1386	1390	1393	rBV2	48605	58623	1.40%	0.166%
15	10.351	1401	1405	1410	rBV	120681	108859	2.60%	0.308%
16	10.639	1449	1454	1464	rBV	2324414	2452706	58.58%	6.948%
17	10.739	1468	1471	1473	rVV2	39267	48892	1.17%	0.139%
18	10.763	1473	1475	1479	rVB3	40125	53364	1.27%	0.151%
19	11.298	1563	1566	1569	rBV2	67990	64140	1.53%	0.182%
20	11.339	1569	1573	1575	rBV	1746181	1687422	40.30%	4.780%
21	11.357	1575	1576	1579	rVB	129739	87494	2.09%	0.248%
22	11.504	1599	1601	1607	rVB	54849	67343	1.61%	0.191%
23	11.869	1660	1663	1666	rBV	58244	53516	1.28%	0.152%
24	11.904	1666	1669	1672	rVB	107678	93306	2.23%	0.264%
25	12.216	1719	1722	1725	rVB	56829	49001	1.17%	0.139%
26	12.321	1736	1740	1745	rBV	55869	55658	1.33%	0.158%
27	12.374	1747	1749	1754	rVB2	52998	58762	1.40%	0.166%
28	12.545	1775	1778	1781	rBV	373490	318128	7.60%	0.901%
29	12.774	1810	1817	1821	rVB	316642	366766	8.76%	1.039%
30	12.827	1824	1826	1835	rVB3	33945	44945	1.07%	0.127%
31	12.927	1838	1843	1846	rBV	3696886	3676766	87.81%	10.416%
32	12.998	1851	1855	1858	rVB3	26437	41879	1.00%	0.119%
33	13.104	1871	1873	1880	rVB	54742	49154	1.17%	0.139%
34	13.457	1929	1933	1938	rBV2	70942	73925	1.77%	0.209%
35	13.545	1943	1948	1951	rVV2	47032	58144	1.39%	0.165%
36	13.615	1957	1960	1964	rVB3	41732	56525	1.35%	0.160%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.774	1985	1987	1992	rVV2	45081	41946	1.00%	0.119%
38	13.815	1992	1994	2002	rVB2	32225	54589	1.30%	0.155%
39	13.939	2003	2015	2016	rBV7	104566	314262	7.51%	0.890%
40	13.974	2016	2021	2024	rVV	1334122	1563746	37.35%	4.430%
41	13.998	2024	2025	2032	rVV	230279	187094	4.47%	0.530%
42	14.068	2032	2037	2048	rVB	351766	463543	11.07%	1.313%
43	14.180	2054	2056	2062	rVB3	56872	62041	1.48%	0.176%
44	14.757	2149	2154	2157	rBV2	36088	42288	1.01%	0.120%
45	14.833	2163	2167	2177	rVB2	37136	54365	1.30%	0.154%
46	14.998	2191	2195	2199	rBV	134898	224946	5.37%	0.637%
47	15.092	2207	2211	2217	rVB3	45614	76736	1.83%	0.217%
48	15.298	2241	2246	2252	rBV	76264	98336	2.35%	0.279%
49	15.357	2252	2256	2262	rBV	85155	115551	2.76%	0.327%
50	15.421	2262	2267	2273	rBV	701311	942445	22.51%	2.670%
51	15.892	2343	2347	2355	rVB2	36851	59034	1.41%	0.167%
52	16.851	2504	2510	2521	rBV3	32165	81870	1.96%	0.232%
53	17.274	2577	2582	2596	rBV3	28377	73342	1.75%	0.208%

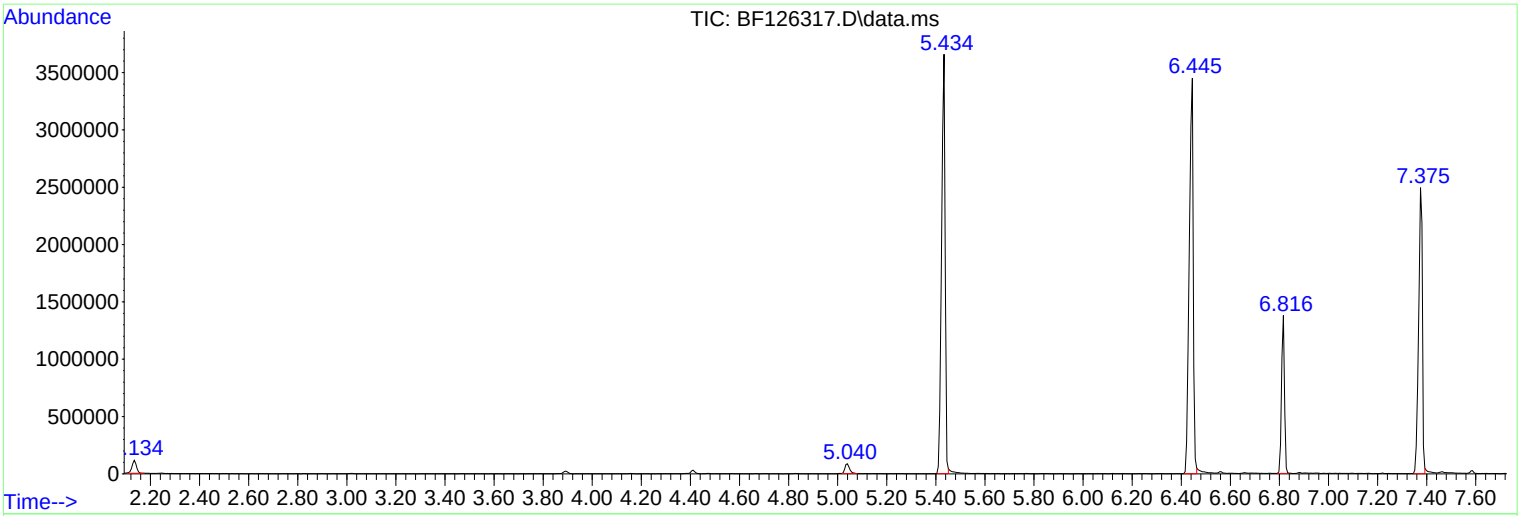
Sum of corrected areas: 35299430

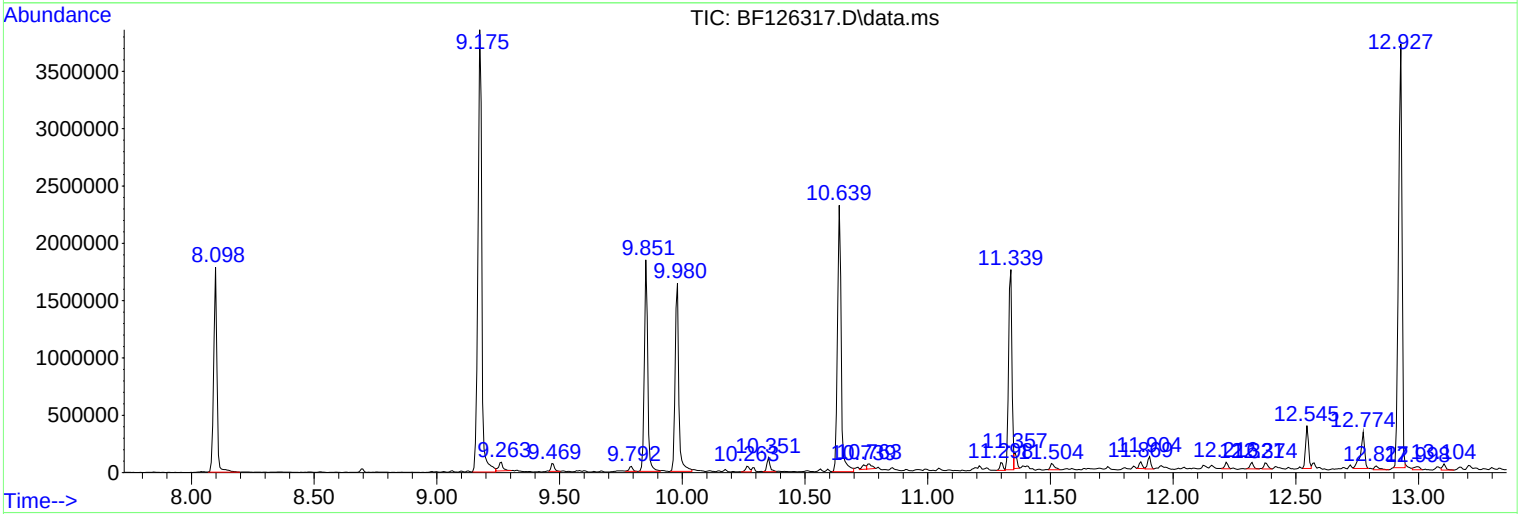
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

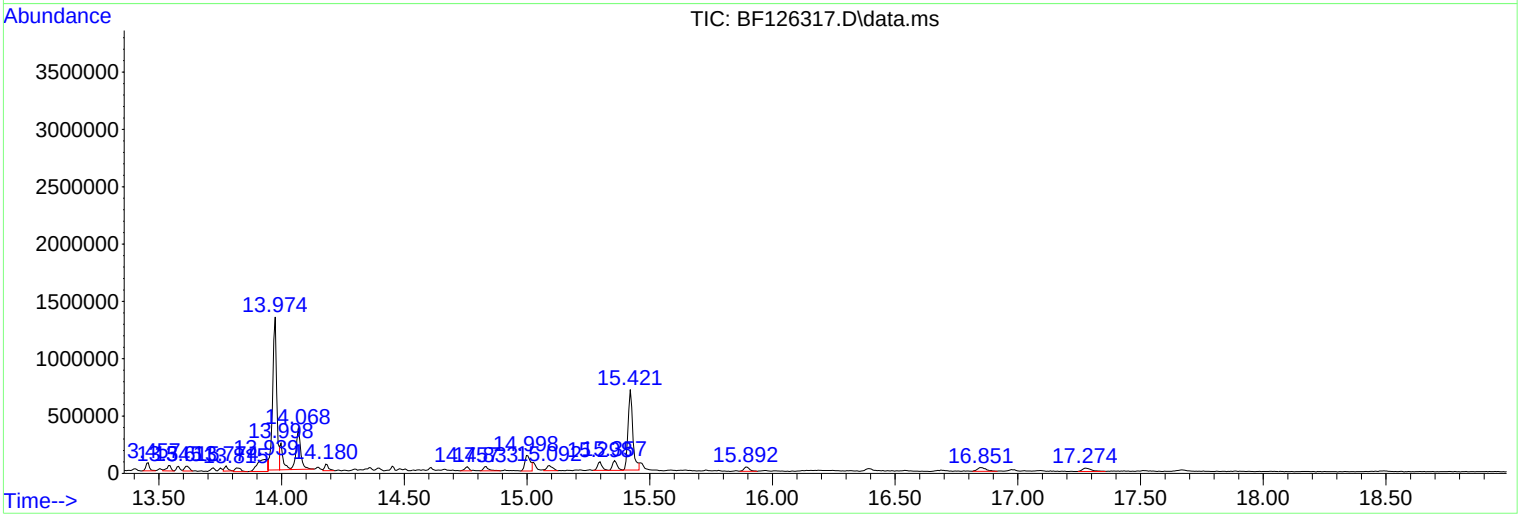
Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

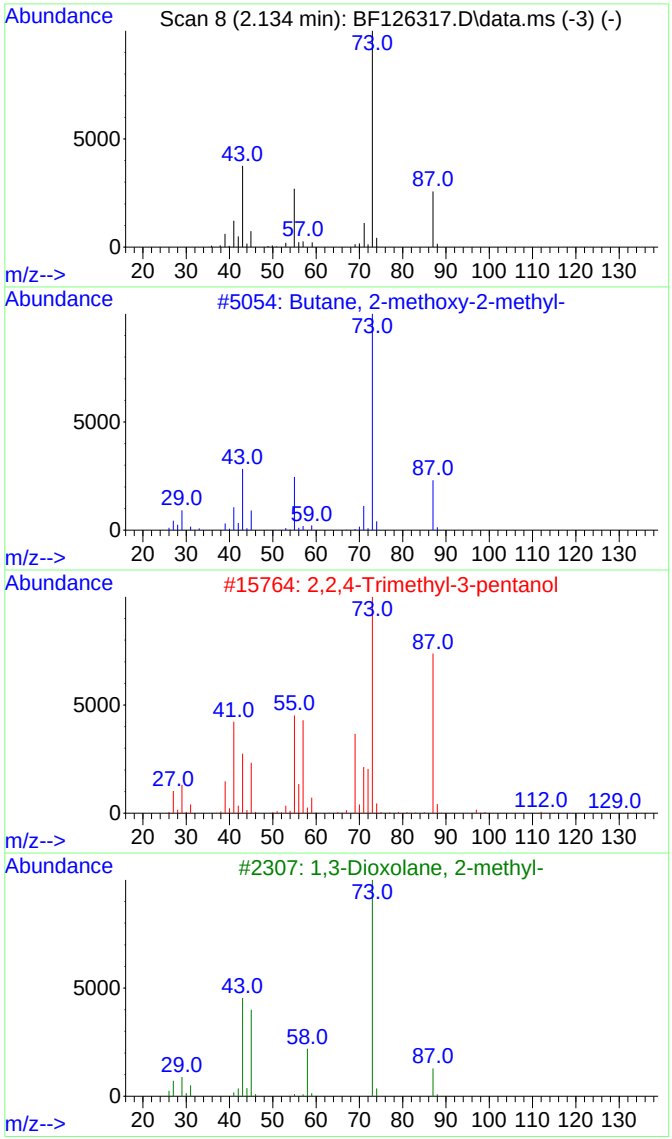
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

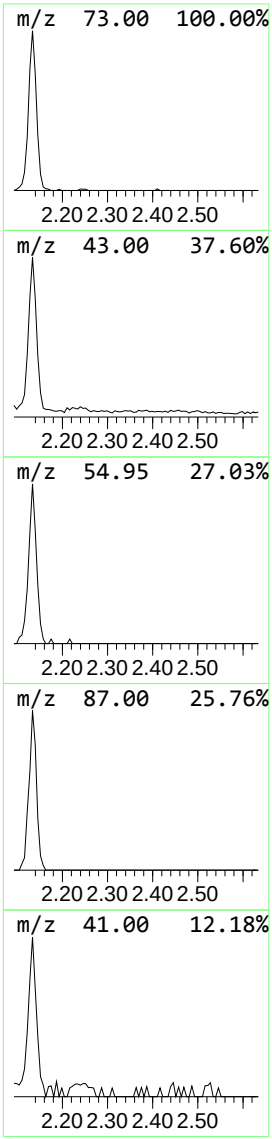
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	2.49 ng	142291	1,4-Dichlorobenzene-d4	6.816

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

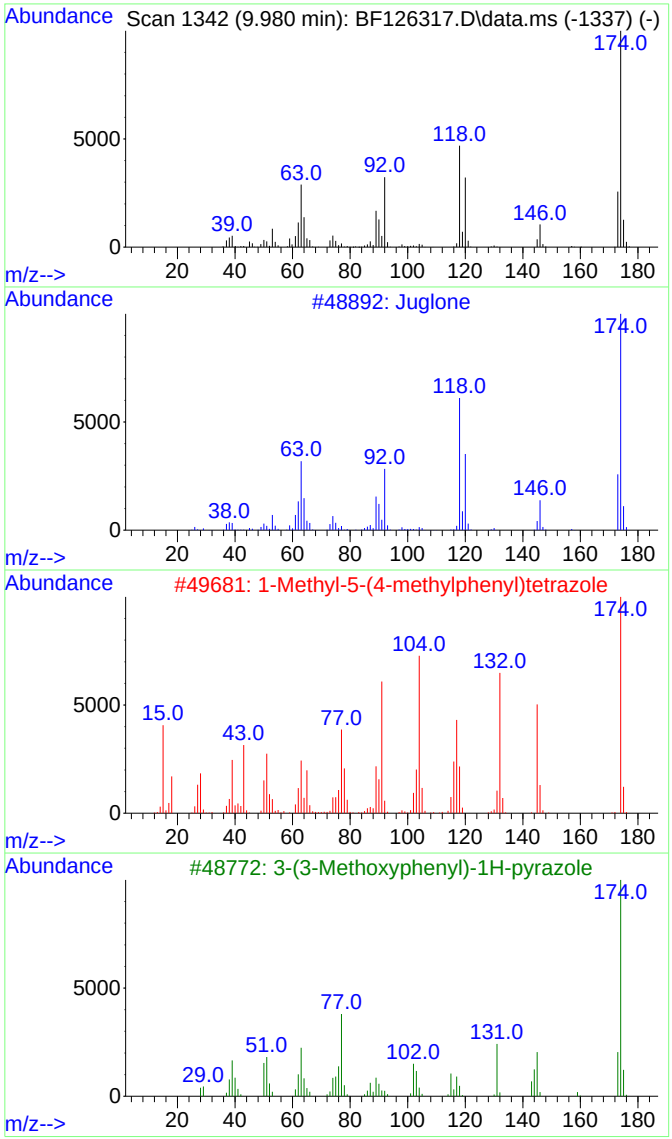
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

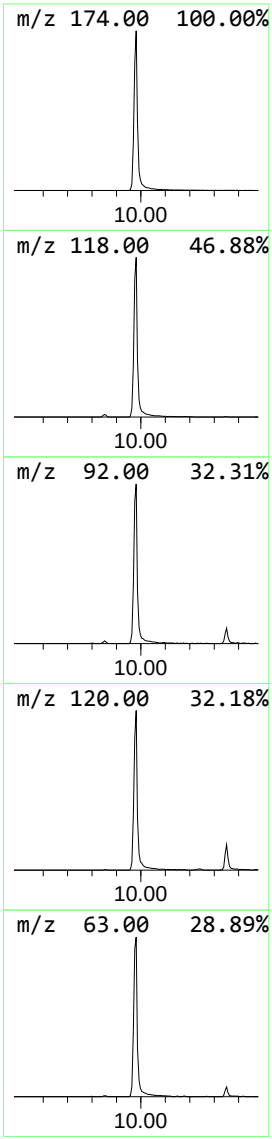
****

Peak Number 2 Juglone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	19.44 ng	1711900	Acenaphthene-d10	9.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone	174	C10H6O3	000481-39-0	98
2	1-Methyl-5-(4-methylphenyl)tetra...	174	C9H10N4	068826-33-5	47
3	3-(3-Methoxyphenyl)-1H-pyrazole	174	C10H10N2O	1000410-63-5	38
4	1-(3-Pyridinylmethyl)-3-piperidi...	275	C16H25N3O	1000469-14-7	38
5	Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

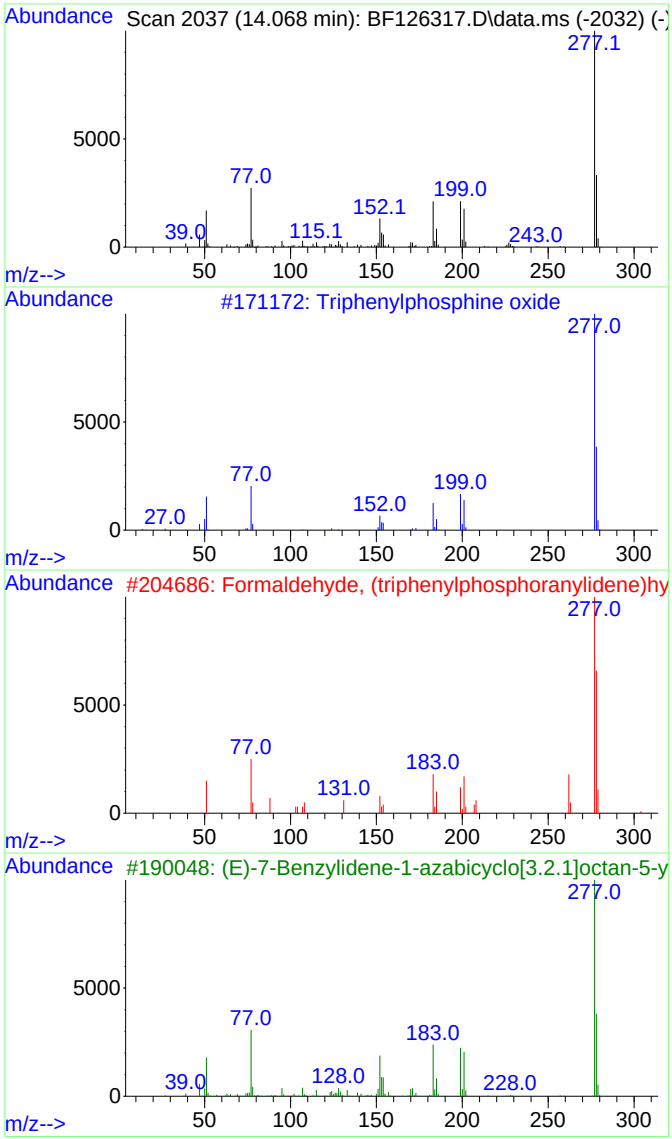
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

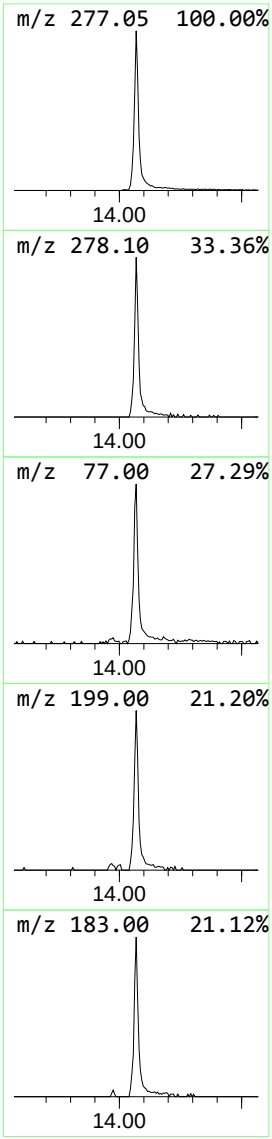
****

Peak Number 3 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	5.93 ng	463543	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
4	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	43
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

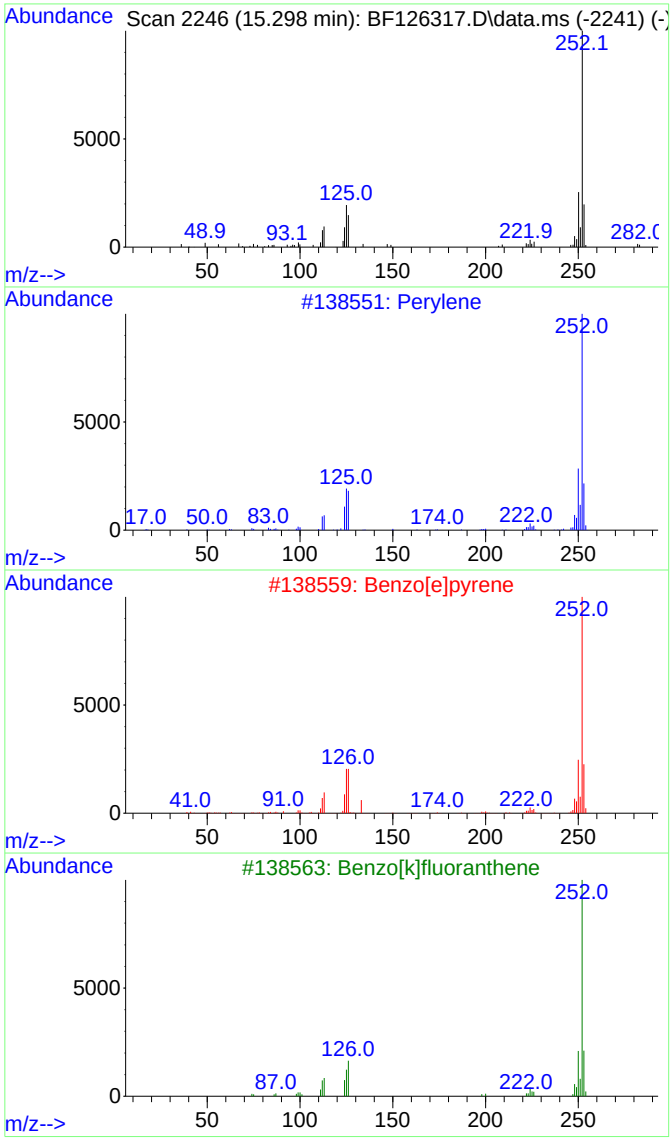
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

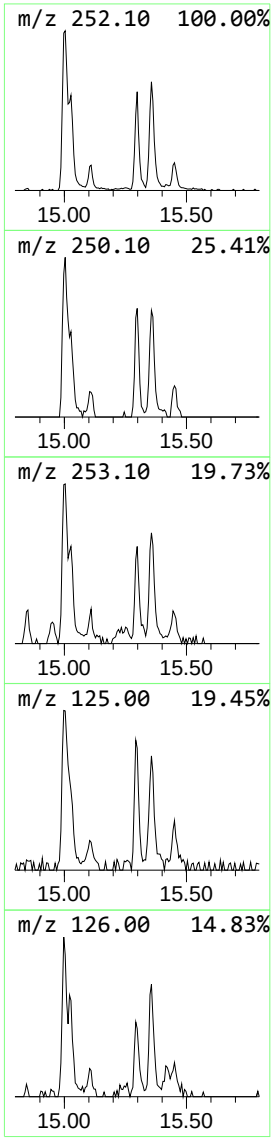
****

Peak Number 4 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.09 ng	98336	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126317.D
Acq On : 22 Dec 2021 1:58
Operator : JU/CG
Sample : M5184-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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
Butane, 2-metho...	2.134	2.5	ng	142291	1	6.816	1141160	20.0
Juglone	9.980	19.4	ng	1711900	3	9.851	1761210	20.0
Triphenylphosph...	14.068	5.9	ng	463543	5	13.974	1563750	20.0
Perylene	15.298	2.1	ng	98336	6	15.421	942445	20.0