LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126264.D
Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2

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: BF126264.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.857	295	301	306	rVB	28541	39995	1.81%	0.219%
2	5.004	492	496	506	rBV	244053	237579	10.74%	1.300%
3	5.292	540	545	547	rBV	55606	54070	2.44%	0.296%
4	5.410	559	565	575	rBV2	649355	758375	34.27%	4.149%
5	5.657	604	607	612	rVB	88188	72237	3.26%	0.395%
6	5.822	632	635	642	rVB2	30043	35529	1.61%	0.194%
7	6.069	674	677	680	rBV2	37581	39424	1.78%	0.216%
8	6.257	705	709	711	rBV2	24177	33824	1.53%	0.185%
9	6.345	721	724	727	rBV2	71240	78776	3.56%	0.431%
10	6.375	727	729	732	rVB	55443	43007	1.94%	0.235%
11	6.428	732	738	743	rBV	723514	685286	30.97%	3.750%
12	6.504	747	751	753	rBV	36179	38003	1.72%	0.208%
13	6.563	756	761	765	rBV3	27052	47510	2.15%	0.260%
14	6.639	771	774	776	rBV	199259	174418	7.88%	0.954%
15	6.657	776	777	780	rVB	114891	69739	3.15%	0.382%
16	6.816	800	804	807	rBV	1837406	1568834	70.90%	8.584%
17	6.875	811	814	818	rBV2	95327	90486	4.09%	0.495%
18	6.969	827	830	833	rBV	51706	47221	2.13%	0.258%
19	6.998	833	835	838	rVB2	62686	53476	2.42%	0.293%
20	7.098	849	852	855	rVB2	67099	70213	3.17%	0.384%
21	7.133	855	858	861	rBV2	49833	60254	2.72%	0.330%
22	7.163	861	863	867	rVB2	50520	43277	1.96%	0.237%
23	7.210	867	871	875	rBV2	74650	75035	3.39%	0.411%
24	7.369	890	898	901	rBV	470723	451567	20.41%	2.471%
25	7.422	901	907	910	rVB	207370	204466	9.24%	1.119%
26	7.463	910	914	918	rVB4	39798	61343	2.77%	0.336%
27	7.610	936	939	941	rBV3	21609	26740	1.21%	0.146%
28	7.722	952	958	960	rBV4	30683	39361	1.78%	0.215%
29	7.739	960	961	965	rVB4	28430	28110	1.27%	0.154%
30	7.857	979	981	985	rVB3	28688	29660	1.34%	0.162%
31	8.098	1017	1022	1025	rBV	2560806	2212729	100.00%	12.107%
32	8.169	1029	1034	1036	rVB	35375	37659	1.70%	0.206%
33	8.698	1119	1124	1128	rVB	28244	27431	1.24%	0.150%
34	9.175	1201	1205	1208	rBV	637605	559310	25.28%	3.060%
35	9.222	1211	1213	1217	rVV2	39987	43160	1.95%	0.236%
36	9.263	1217	1220	1224	rVB	33346	31162	1.41%	0.171%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126264.D
Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2

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	9.851	1315	1320	1331	rBV	2343474	2135116	96.49%	11.682%
38	10.398	1410	1413	1417	rVB	37187	36000	1.63%	0.197%
39	10.633	1449	1453	1458	rBV	261454	237574	10.74%	1.300%
40	10.780	1472	1478	1483	rVB3	27944	48498	2.19%	0.265%
41	11.210	1543	1551	1553	rBV4	30256	43115	1.95%	0.236%
42	11.245	1553	1557	1560	rVB4	24671	36754	1.66%	0.201%
43	11.333	1568	1572	1575	rBV	1962235	1806971	81.66%	9.887%
44	11.357	1575	1576	1579	rVV	285650	172218	7.78%	0.942%
45	11.410	1582	1585	1588	rVB	48549	49675	2.24%	0.272%
46	11.833	1654	1657	1660	rBV	40171	36694	1.66%	0.201%
47	11.863	1660	1662	1667	rBV	140240	149470	6.76%	0.818%
48	11.945	1673	1676	1679	rBV	58678	65102	2.94%	0.356%
49	12.039	1689	1692	1695	rVB4	21606	26473	1.20%	0.145%
50	12.086	1695	1700	1703	rBV4	48993	52852	2.39%	0.289%
51	12.198	1716	1719	1721	rBV	71070	59687	2.70%	0.327%
52	12.286	1728	1734	1737	rBV	183011	176718	7.99%	0.967%
53	12.363	1744	1747	1750	rBV	121787	116132	5.25%	0.635%
54	12.421	1755	1757	1763	rVB4	27663	46991	2.12%	0.257%
55	12.545	1774	1778	1781	rBV	307759	258808	11.70%	1.416%
56	12.592	1781	1786	1791	rVV	228402	214670	9.70%	1.175%
57	12.651	1793	1796	1801	rBV6	39016	53962	2.44%	0.295%
58	12.774	1811	1817	1820	rBV	250690	282244	12.76%	1.544%
59	12.915	1838	1841	1849	rVB	456422	412135	18.63%	2.255%
60	13.104	1870	1873	1877	rVB2	57863	61795	2.79%	0.338%
61	13.168	1880	1884	1886	rVV2	52380	53228	2.41%	0.291%
62	13.204	1886	1890	1899	rVV4	59844	92243	4.17%	0.505%
63	13.968	2015	2020	2023	rBV2	1439565	1530709	69.18%	8.375%
64	14.068	2032	2037	2046	rBV	461004	509511	23.03%	2.788%
65	14.757	2152	2154	2156	rBV2	38631	33818	1.53%	0.185%
66	14.998	2192	2195	2198	rBV2	86155	133048	6.01%	0.728%
67	15.292	2242	2245	2250	rVB2	76687	90309	4.08%	0.494%
68	15.351	2253	2255	2259	rVB	63922	65341	2.95%	0.358%
69	15.415	2262	2266	2270	rBV2	870858	1019210	46.06%	5.577%

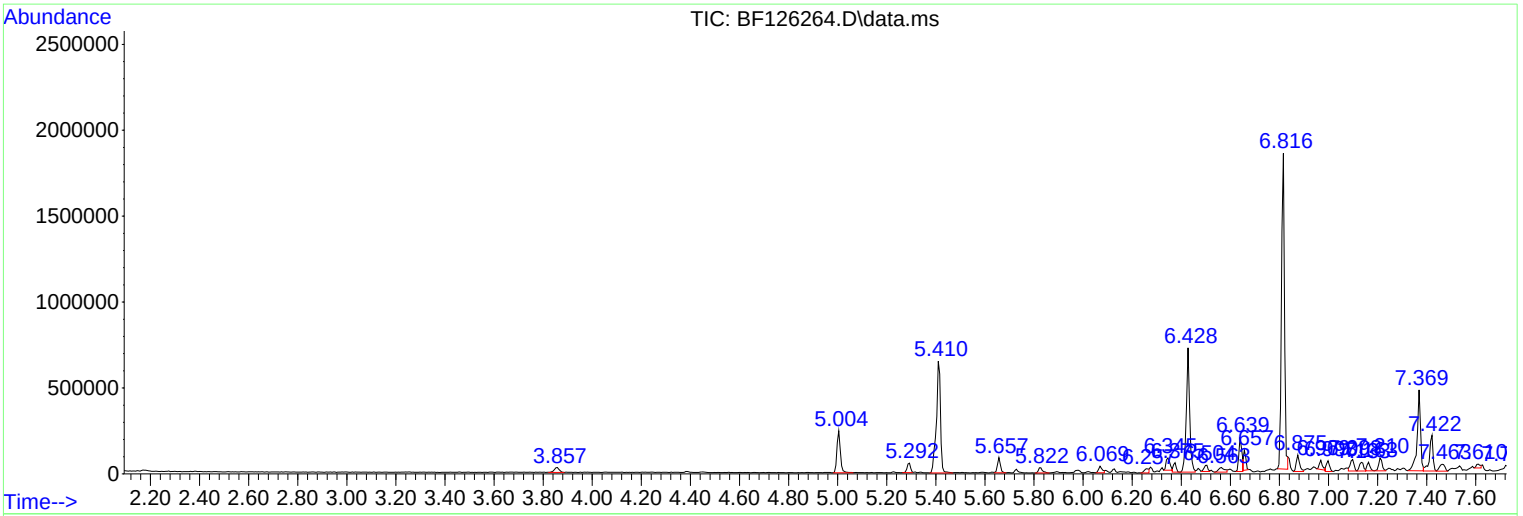
Sum of corrected areas: 18276337

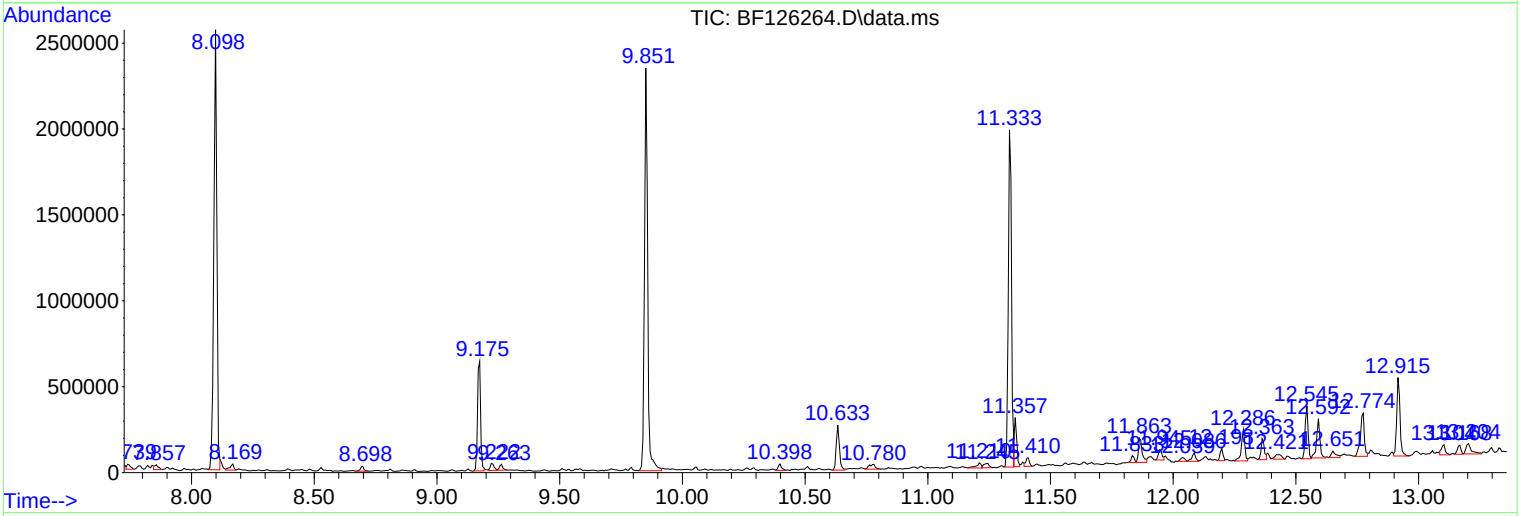
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126264.D
Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

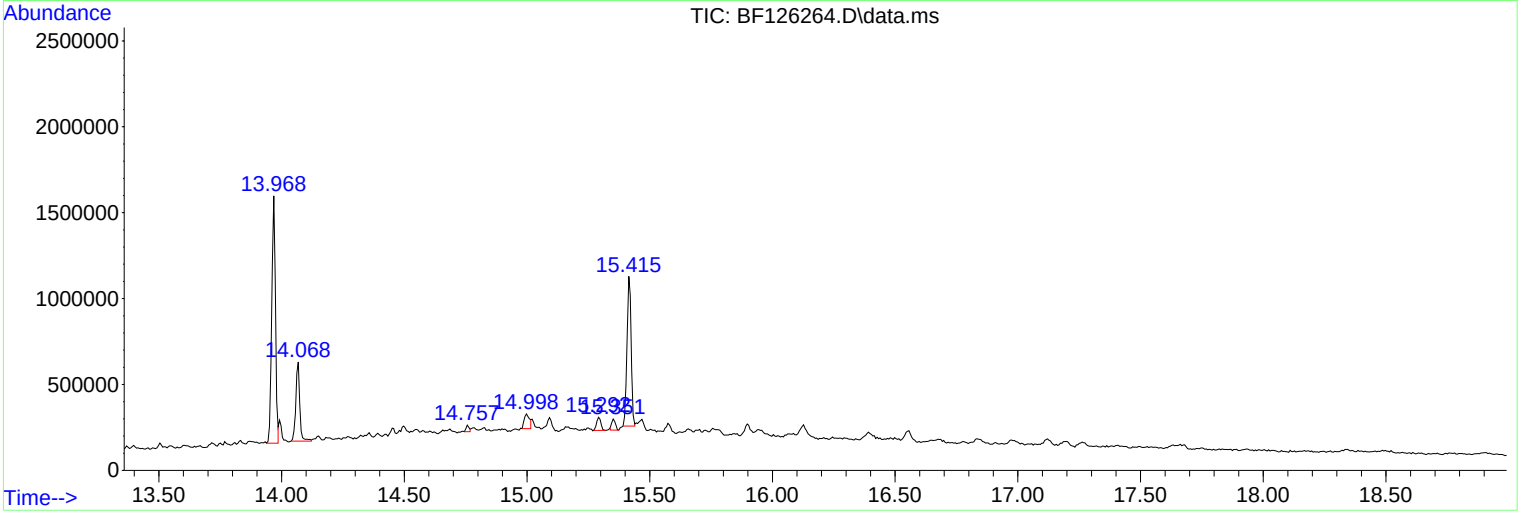
Instrument :
BNA_F
ClientSampleId :
A2

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\BF121821\
Data File : BF126264.D
Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2

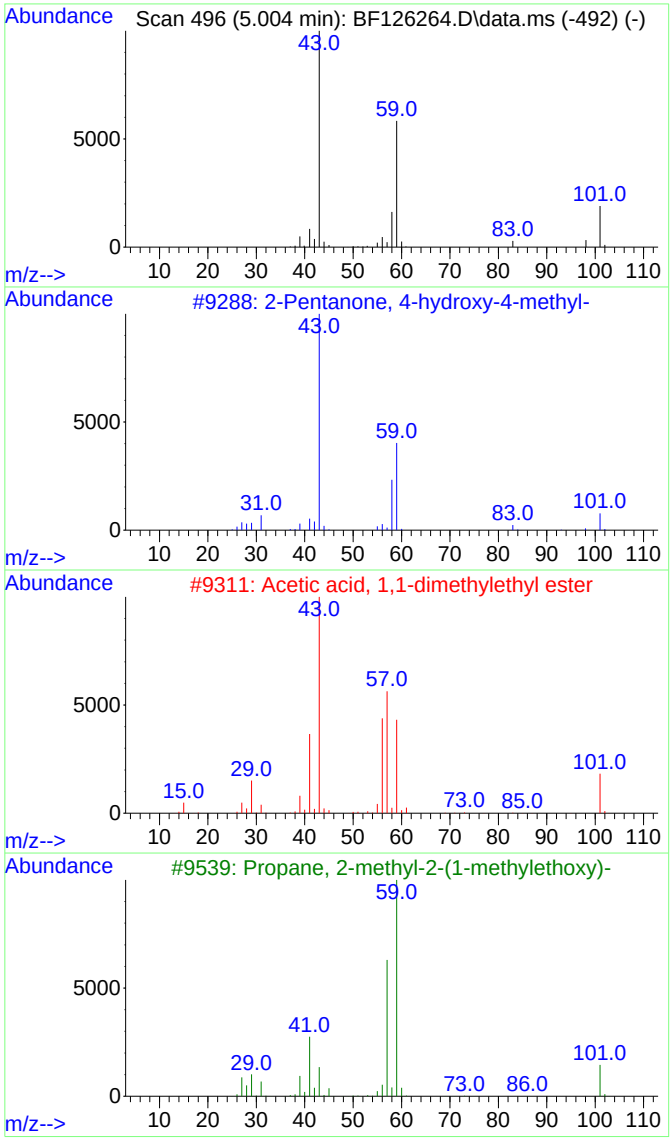
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

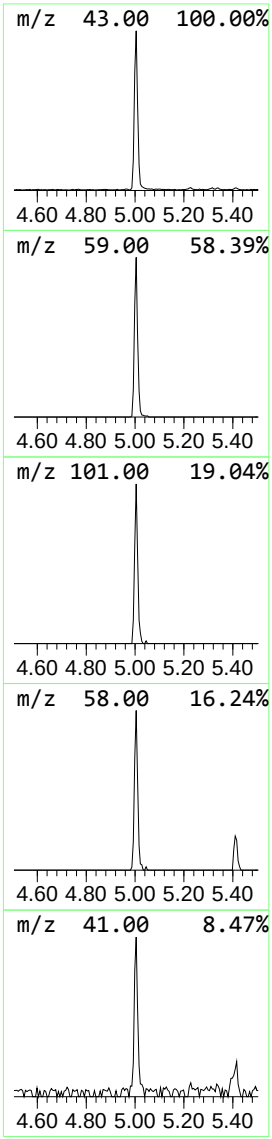
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	3.03 ng	237579	1,4-Dichlorobenzene-d4	6.816

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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126264.D
Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2

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

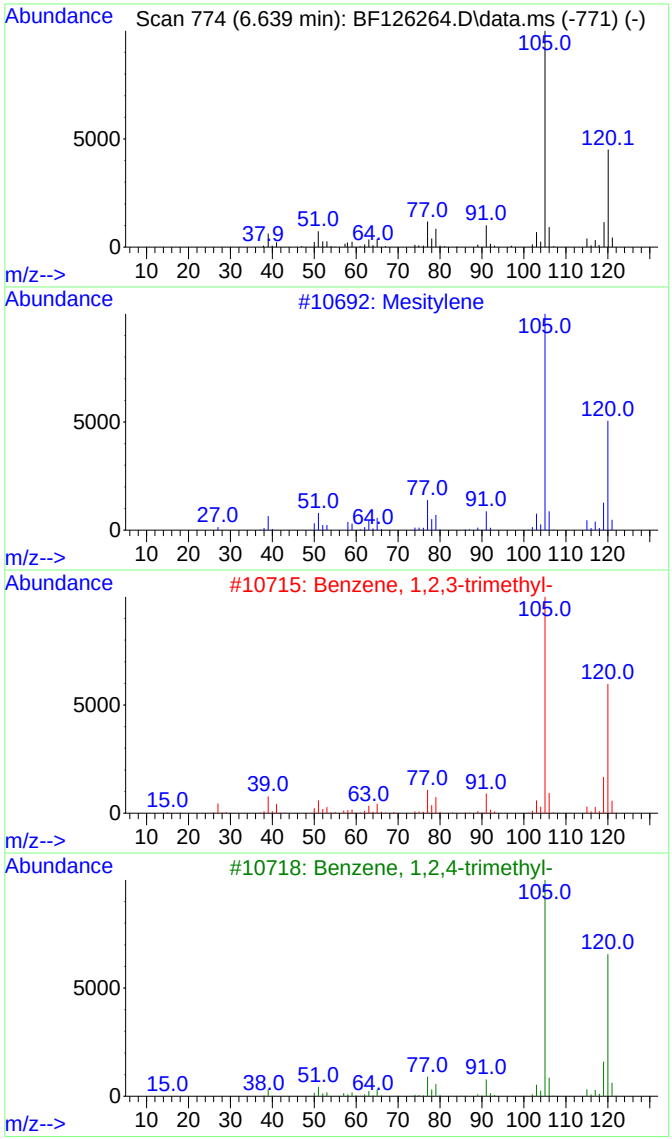
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

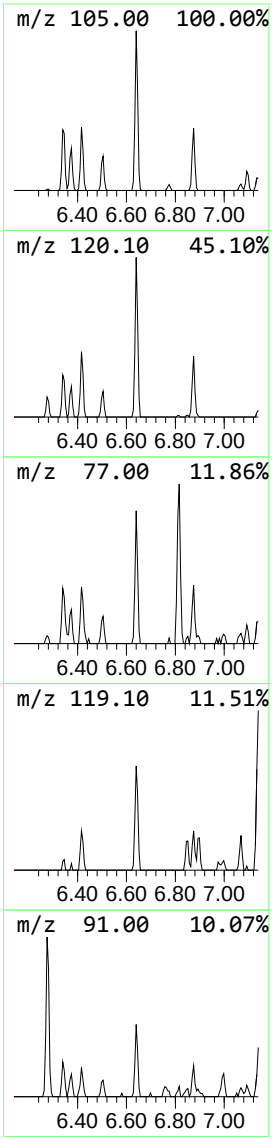
****

Peak Number 2 Mesitylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.639	2.22 ng	174418	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126264.D
Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2

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

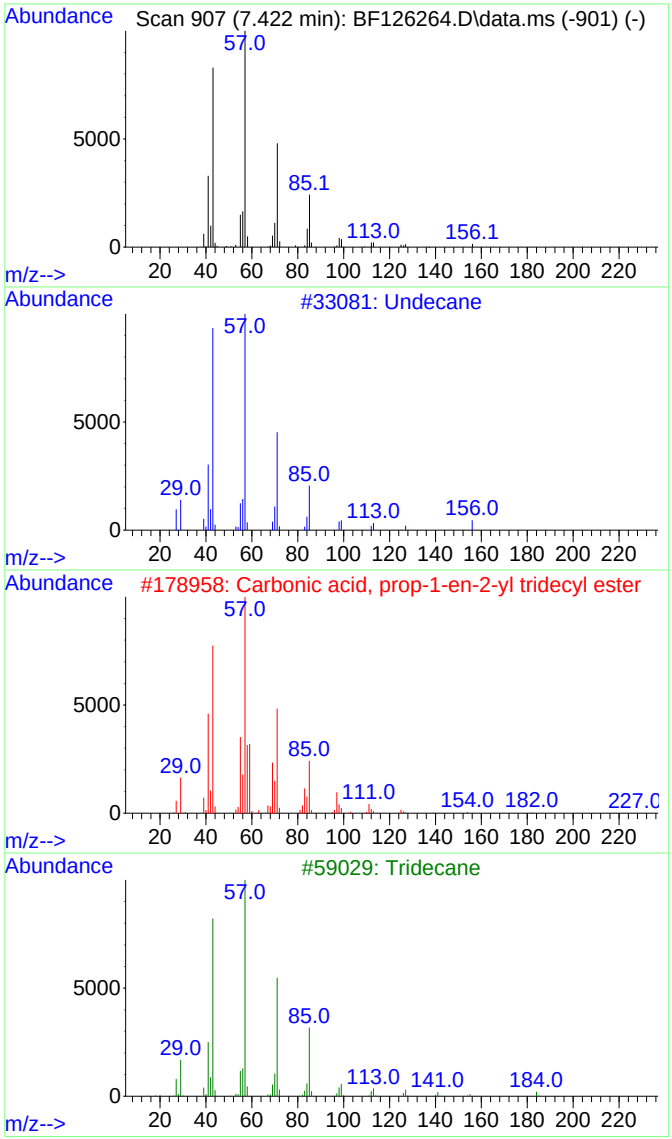
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

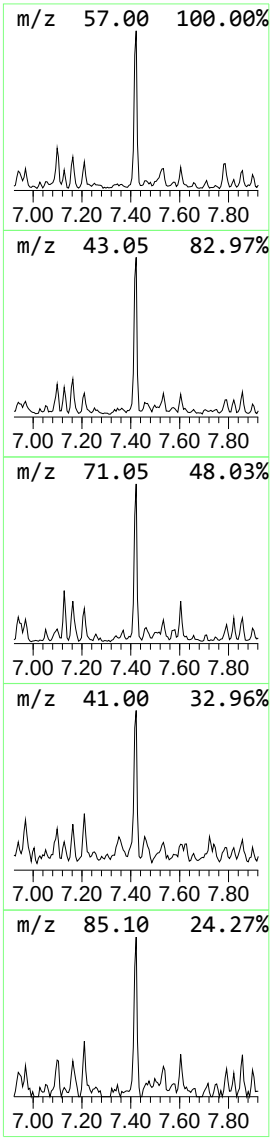
****

Peak Number 3 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.422	2.61 ng	204466	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	91
2	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	86
3	Tridecane	184	C13H28	000629-50-5	83
4	Hexadecane	226	C16H34	000544-76-3	78
5	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	78





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Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2

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

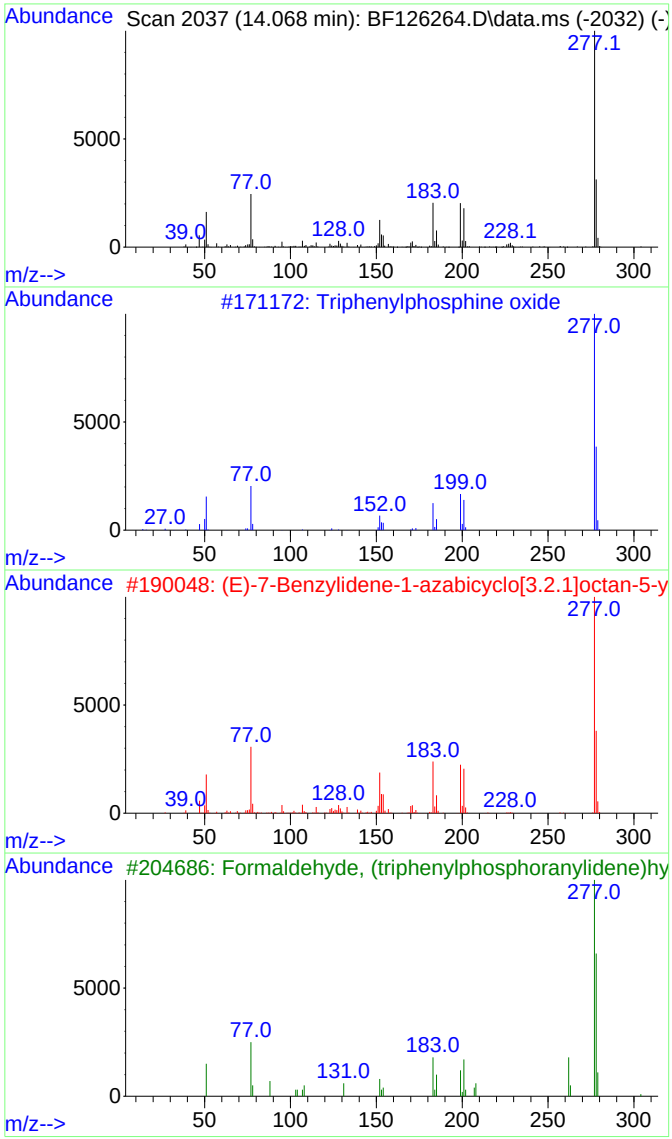
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

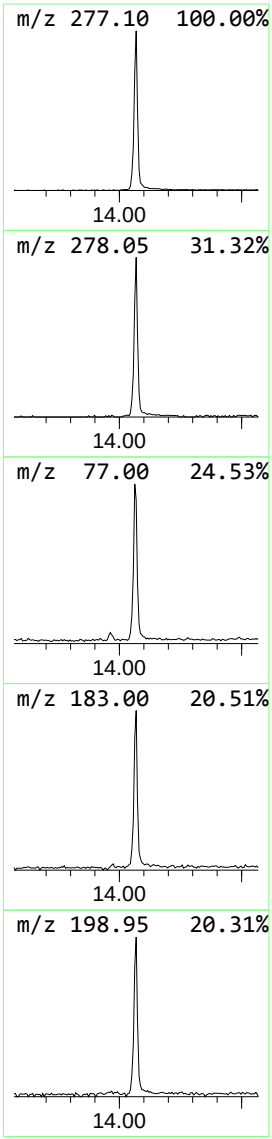
****

Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	6.66 ng	509511	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	81
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126264.D
Acq On : 18 Dec 2021 20:22
Operator : JU/CG
Sample : M5142-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2

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
2-Pentanone, 4-...	5.004	3.0	ng	237579	1	6.816	1568830	20.0
Mesitylene	6.639	2.2	ng	174418	1	6.816	1568830	20.0
Undecane	7.422	2.6	ng	204466	1	6.816	1568830	20.0
Triphenylphosph...	14.068	6.7	ng	509511	5	13.968	1530710	20.0